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Sampling Strategies for Water Quality in the Great Lakes

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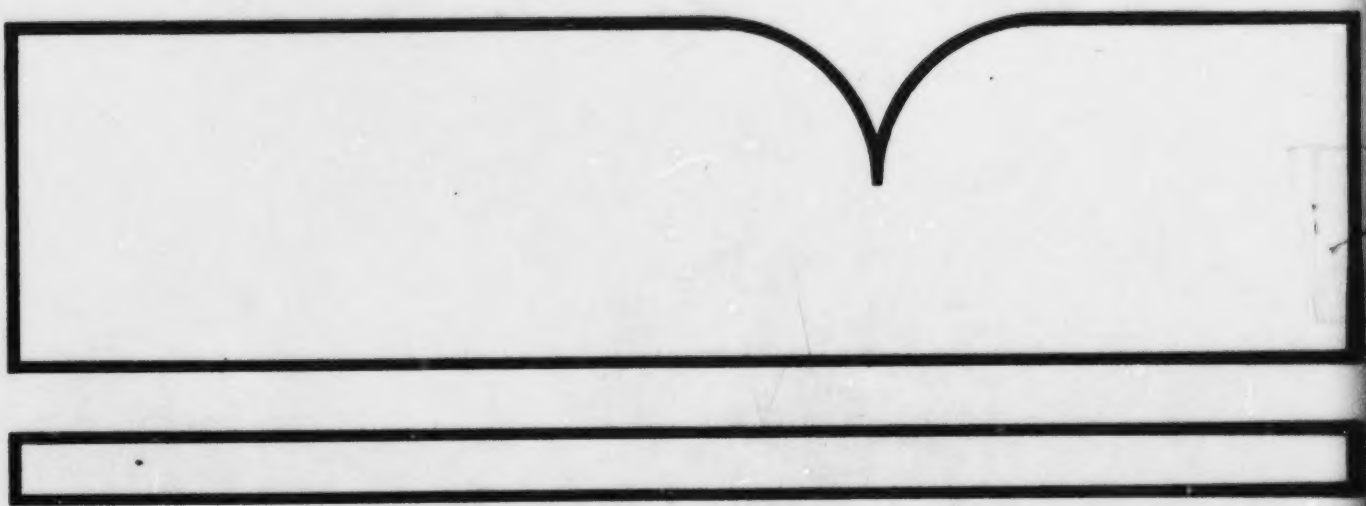

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The major goal of this project was to investigate the potential applications of Kalman filtering and modern optimization techniques to the design of sampling strategies for water quality in the Great Lakes. Two representative problems of general limnological interest with considerably different characteristics were studied. The first problem concerns sampling requirements for long-term trend detection of chloride and total phosphorus concentrations in Lake Michigan. A minimum-cost sampling strategy has been determined in association with the Kalman filter and mathematical models that can detect changes of 1.0 mg Cl/ℓ and 1.0 μg P/ℓ in Lake Michigan with 90 percent probability. The cost of this sampling program is considerably less than monitoring programs designed without benefit of mass balance models and Kalman filter data processing. An investigation was conducted to determine the sensitivity of the optimal cost to the accuracy of the mass balance model parameters. It is concluded that the calculated sampling cost is most sensitive to the variance in the apparent phosphorus settling velocity, not as sensitive to the accuracy of laboratory analyses, and rather insensitive to the accuracy of the effective flow at the Straits of Mackinac and atmospheric loads. The second problem concerns the potential applicability of Kalman filtering techniques for concentration estimation and parameter identification for a phytoplankton and nutrient cycling model for Saginaw Bay.

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FOREWORD

One of the goals of the International Surveillance Program for the Great Lakes is to detect long-term changes in the concentration of various parameters in each of the lakes. In order for this program to be successful, data of sufficient quality and quantity must be provided so that trends can be accurately assessed. However, each additional sample collected increases the cost of the program. There is, therefore, a trade-off between accuracy and cost and a sampling strategy must be identified that will obtain the necessary accuracy at the minimum possible cost.

This report is the result of an effort to use basic ideas from control theory and statistics to develop a methodology for identifying optimum sampling strategies. Besides the applications included in this report, this research effort has stimulated further work on different parameters and space and time scales.

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ABSTRACT

The major goal of this project was to investigate the potential applications of Kalman filtering and modern optimization techniques to the design of sampling strategies for water quality in the Great Lakes. Two representative problems of general limnological interest with considerably different characteristics were studied. The first problem concerns sampling requirements for long-term trend detection of chloride and total phosphorus concentrations in Lake Michigan. A minimum-cost sampling strategy has been determined in association with the Kalman filter and mathematical models that can detect changes of 1.0 mg Cl/ℓ and 1.0 μg P/ℓ in Lake Michigan with 90 percent probability. The cost of this sampling program is considerably less than monitoring programs designed without benefit of mass balance models and Kalman filter data processing. An investigation was conducted to determine the sensitivity of the optimal cost to the accuracy of the mass balance model parameters. It is concluded that the calculated sampling cost is most sensitive to the variance in the apparent phosphorus settling velocity, not as sensitive to the accuracy of laboratory analyses, and rather insensitive to the accuracy of the effective flow at the Straits of Mackinac and atmospheric loads.

The second problem concerns the potential applicability of Kalman filtering techniques for concentration estimation and parameter identification for a phytoplankton and nutrient cycling model for Saginaw Bay. The approach has been used to obtain estimates of the accuracy of model-predicted phytoplankton concentrations in Saginaw Bay as a function of the uncertainty associated with model parameters and initial conditions. It has been determined that the accuracy of uncalibrated model predictions is limited and depends on the location within the bay. However, the accuracy of the predictions can be improved if the uncertainties of the model parameters and initial conditions can be reduced by laboratory experiments or the availability of field data. Examples are presented that show how suboptimal sampling strategies can be developed and used to increase the predictive capabilities of uncalibrated phytoplankton models in Saginaw Bay.

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SECTION 1

INTRODUCTION

The determination of effective sampling strategies for estimating water quality in lakes depends upon many factors such as seasonal and annual variations, spatial variations, quality of the measurement techniques, accuracy of the estimates desired, and economic feasibility. Because of these many factors, a computer based approach could prove to be a very useful tool in the design of sampling strategies for water quality in the Great Lakes. This research is concerned with developing such a computer based approach and demonstrating its feasibility on two different types of problems.

The basic mathematical approach employed in the solution of these problems is an information processing technique known as Kalman filtering. This technique couples knowledge of the quality of the measurement procedures, mathematical models of the biochemical processes, and the adequacy of these measurements and models (for example, variances associated with measurement and model noise) to determine best estimates of the concentrations of the water quality variables and the variance of the estimates. In addition, if the number of variables involved is not too large, automatic computer-based optimization techniques can be employed to define optimal sampling strategies.

Mathematical models of long-term (30 years) phosphorus and chloride concentration changes in Lake Michigan are developed along with variances associated with these models in Section 5. This model and proposed monitoring programs for the lake can be used to develop an optimal sampling strategy that can be completely determined economically on a large computer. This allows an extensive sensitivity study of the various factors that affect the measurement program. A modified LAKE 1 (Thomann et al., 1975) model is employed in Section 6 for the determination of a short term (1 year) measurement strategy for phytoplankton, zooplankton, and nutrients in Saginaw Bay. The resultant model contains eight concentration variables in each of five segments. Furthermore, thirty-five additional differential equations are used to improve some of the model parameter estimates. As a result, a system has evolved that is too large for economical automatic computer optimization. However, analysis of the variances developed by the Kalman filter makes it possible to assess the adequacy of the model predictions and to develop suboptimal measurement strategies.

A brief heuristic introduction to the Kalman filter is presented in Section 4. More details concerning the mathematical procedures employed to

develop the Kalman filter and to derive the minimum-cost sampling strategy subject to the variance constraints are presented in Appendix A and in DePalma (1977). The reader interested only in the water quality applications may proceed directly to Sections 5 and 6.

SECTION 2

CONCLUSIONS

The results of this study indicate that Kalman filtering techniques can be applied effectively to assist with the design of limnological and water quality sampling programs in the Great Lakes. This conclusion is based on encouraging results obtained for two demonstration problems. First, the Kalman filter and optimization procedures have been used to design an optimal long-term monitoring program for chloride and total phosphorus in Lake Michigan. This sampling program detects concentration changes of 1 mgCl/ℓ and 1 μgP/ℓ with 90 percent confidence and is considerably less expensive than sampling programs suggested without benefits of mass balance models and Kalman filtering. The procedures applied to this problem can also be used to study the value of mass balance models for trend detection. As model parameter uncertainties decrease, the model becomes more accurate and useful, and actual field monitoring requirements and costs decrease. Preliminary calculations suggest that it may be appropriate to invest research funds to improve analytical techniques for total phosphorus and to obtain better estimates for the rate of phosphorus loss to the sediments.

Kalman filtering and state estimation techniques have been used to calculate the uncertainty associated with phytoplankton model predictions as a function of the accuracy of model parameters and initial conditions. Preliminary calculations indicate that errors in uncalibrated model predictions of phytoplankton in Saginaw Bay can be significant even if it is assumed that the structure and nature of the system equations are perfect. Thus, before accurate predictions can be made, it is necessary to improve estimates of the model parameters with field monitoring or laboratory research programs or to supplement model predictions with measured data to update state estimates using the Kalman filter. These results have direct significance when models are used for planning purposes such as predicting the impact of nutrient control programs in the Great Lakes.

SECTION 3

RECOMMENDATIONS

This study has determined an optimal, minimum-cost sampling strategy for long-term trend detection of chloride and total phosphorus in Lake Michigan. This strategy involves limited tributary samples and lake monitoring only for those years when concentrations must be determined. It is recommended that this sampling schedule be initiated if the only goal of the measurement efforts is that of trend detection. Sampling requirements for other goals (such as to define annual nutrient and plankton cycles) would obviously have different characteristics. In such cases, it may be possible to again define the most efficient sampling program if the system dynamics can be formulated to accommodate Kalman filtering methodology. Finally, it is recommended that the optimal sampling be recomputed if research results or field data become available in the future that would allow more accurate statistical assessment of the model parameters and processes.

The Kalman filtering and state estimation techniques applied in this study have been used to estimate the uncertainty of phytoplankton model predictions in Saginaw Bay as a function of the accuracy of model parameters and initial conditions. However, error propagation for only seven parameters (from a total of twenty) has been studied because of funding and time limitations of this project. Furthermore, the error covariance calculations depend on the adequacy of a linear approximation of the system state equations. It is recommended that the adequacy of this approximation and the numerical methods employed be evaluated further before the results of the calculations presented in this report are incorporated in water quality planning projects.

SECTION 4

INTRODUCTION TO KALMAN FILTERING

INTRODUCTION

The Kalman filter was derived by Kalman (1960) and Kalman and Bucy (1961) and has had considerable application in aerospace engineering and, more recently, to some problems concerned with water quality (Moore, 1971; Beck and Young, 1976). In order to simplify the presentation, this section describes the Kalman filter equations for a scalar system in which the water quality variable is measured at distinct measurement times and the water quality model is a differential equation. Complete derivation of the equations for other cases may be found in Gelb (1974), Jazwinski (1970), and Sage and Melsa (1971), among others. Appendix A gives the Kalman filter equations for a general discrete dynamic model for cases where only some of the water quality variables are measured along with the method of employing the filter in the determination of minimum cost measurement strategies for a given level of required accuracy.

KALMAN FILTER EQUATIONS

The Kalman filter is an information processing technique that combines a dynamic model and measurements to produce an improved estimate of the state of the system (for example, the concentrations of the water quality variables). If an adequate dynamic model for the system does not exist, then standard statistical techniques can be employed, using only the concentration measurements, to estimate the state of the system. Thus, Kalman filtering is mainly applicable when some type of dynamic model of the system is available. However, even dynamic models that give only seasonal or annual trends usually justify the use of the Kalman filter.

Suppose that a mathematical model of the biological and chemical interactions is a system of differential equations

$$\dot{x} = f(t,x) + w(t) \tag{4.1}$$

where $x(t)$ is a n-vector that represents the concentration of the water quality variables at time t (for example $x_1(t)$ = phytoplankton concentration at time t), $f(t,x)$ is a function that describes the known rate of change of x (for example, f contains the advective and dispersive transport, loadings, and kinetic coefficients), and $w(t)$ is the error in the model at time t.

One of the most difficult problems in mathematical modeling is the quantification of the error term w(t) because this term is an indicator of the value of the model. If w(t) could be characterized completely, then, it could become part of the f(t,x) term. For most applications, it is only possible to statistically characterize the term w(t), which is usually assumed to be zero-mean, white noise with variance Q(t). The white noise assumption is conservative because it implies no time correlation in the model error w(t). The accuracy of the dynamic equations is implied by the magnitude of Q. Relatively large values of Q imply that f(t,x) is relatively inaccurate. Quantitative determination of the true value of Q is very difficult, if not impossible. Thus, in most applications conservative upper bounds are employed as estimates for Q. As an alternative, liberal estimates for Q (that is, when Q = 0) give the estimation capabilities of a perfect model. Note that w(t) includes any inaccuracies associated with the forcing functions of the system.

In addition to statistically characterizing the error term in Equation (4.1), it is also necessary to statistically characterize the initial conditions of the system variables at time equal to zero, t_0. Before the Kalman filter can be employed, values for the mean ($\hat{x}_0$) and variance (P_0) of the initial state (for example, the concentrations of the water quality variables) must be available at a time prior to the first measurement.[1]

The problems solved in this report involve discrete sampling (as opposed to continuous monitoring), therefore the measurement process can be described as

$$y(t_i) = x(t_i) + v(t_i) \quad (i = 1,2,\ldots,N) \tag{4.2}$$

where $y(t_i)$ is the measured value of x at t_i, $v(t_i)$ is the error in the measurement at t_i, and N is the number of measurements. Appendix A discusses cases where only some of the concentrations are measured. It is assumed that v has a mean value of zero and a variance R. Typically, the measurement process is relatively well known and can be characterized accurately.

Given the information in Equations (4.1) and (4.2) suppose it is desired to estimate the concentration of a variable in a scalar system at $t_1 > t_0$ (that is, at the first measurement time). This estimation will utilize both the model prediction and measurement at t_1. The Kalman filter is used to calculate this estimate in two stages. The first stage involves a prediction of x at t_1 before the actual measurement is taken, which will be denoted by $\hat{x}(t_1^-)$, and the variance associated with this estimate is denoted by $P(t_1^-)$.

The predicted value of the concentration is simply the integration of Equation (4.1) with w(t) = 0 from t_0 to t_1 with $\hat{x}(t_0) = \hat{x}_0$. That is, integrate

[1] In this report, x refers to true values of the state variables, whereas $\hat{x}$ refers to estimated values.

$$\dot{\hat{x}} = f[t,\hat{x}(t)],\ \hat{x}(t_0) = \hat{x}_0 \tag{4.3}$$

to t_1. This is equivalent to simply using the model to calculate concentrations at t_1 under the assumption that the model is perfect. The variance of the resultant concentration at t_1 for the scalar case is denoted as $P(t_1^-)$ and is calculated approximately by integrating

$$\dot{P} = 2AP + Q \tag{4.4}$$

with $P(t_0) = P_0$ from t_0 to t_1 where

$$A = \frac{\partial f[t,x]}{\partial x}\Big|_{(t,\hat{x}(t))}. \tag{4.5}$$

This is called the sensitivity of the dynamic equation. This equation is based on the theory of stochastic estimation and has been derived by Jazwinski (1970) and others. If $f(t,x)$ is linear in x, then Equation (4.4) gives the true variance of x. Other approximations for P are discussed in Appendix A. The approximation of Equations (4.3-4.5) is known as the extended Kalman filter.

Equation (4.4) is used to calculate the accuracy of the prediction based on the characteristics of the system (for example, transport and kinetics) and the model error. If the first term in Equation (4.4) is positive (for example, during rapid concentration increases), then the associated variance increases between measurements, and initial condition errors are magnified as time increases. Conversely, if concentrations are decreasing rapidly, the first term in Equation (4.4) will be negative, and the accuracy of the estimate could actually increase. A simple example will be presented later in this section to illustrate this effect. The second term in Equation (4.4) (Q) is always positive. Thus, it can only cause the accuracy of the estimate to deteriorate as time increases.

Integration of Equations (4.3) and (4.4) from t_0 to t_1 is the first stage of the Kalman filter, and $x(t_1^-)$ and $P(t_1^-)$ are the results. The second stage involves processing the measurement $y(t_1)$, as described by Equation (4.2), to develop an improved estimate of the concentration at t_1, which is denoted by $x(t_1^+)$ and the associated concentration variance $P(t_1^+)$. The Kalman filter equations for the scalar case for this stage are

$$\hat{x}(t_1^+) = \hat{x}(t_1^-) + K(t_1)[y(t_1) - \hat{x}(t_1^-)] \tag{4.6}$$

$$P(t_1^+) = [1 - K(t_1)]P(t_1^-) \tag{4.7}$$

$$K(t_1) = P(t_1^-)[P(t_1^-) + R_1]^{-1} \tag{4.8}$$

where $K(t_1)$ is called the Kalman Gain. K is called a gain because, by analogy with feedback gain in electronics, it determines how much weighting is given to the measurement in developing the estimate for the concentration at time t_1^+. These equations have been developed by Jazwinski (1970) and others and are based on determining a minimum variance estimate for the con-

centrations using information from both the mathematical model and imperfect measurements.

It is instructive to consider two special extreme cases of Equations (4.6-4.8). First, suppose that the measurement at t_1 is much more accurate than the estimate generated by the model from t_0 to t_1 (that is, $P(t_1^-)$ is much greater than R_1). Then, from Equation (4.8) the Kalman Gain approaches one, and from Equation (4.6) $\hat{x}(t_1) \approx y(t_1)$. Thus, the new information provided by the model has little significance. Also, note that from Equation (4.7) the associated variance for this case is approximately zero. Of course, $P(t_1^+)$ equals zero only for a perfect measurement defined by $R_1 = 0$.

Next, consider the case where the measurement is poor and not as accurate as the value predicted by the model (that is, $P(t_1^-)$ is much less than R_1). Then, from Equation (4.8) the Kalman Gain approaches zero, and $\hat{x}(t_1^+) \approx \hat{x}(t_1^-)$. In this case, the calculated concentration t_1^+ is approximately the value determined by the model, or in the limit as $R_1 \to \infty$ it is as if no measurements were conducted. Note that Equation (4.7) implies $P(t_1^+) \approx P(t_1^-)$, which must be the case if $\hat{x}(t_1^+) \approx \hat{x}(t_1^-)$ with R_1 relatively large.

The remaining measurements $y(t_2),\ldots,y(t_n)$ are processed by simply proceeding in the same manner as the two stages noted above. That is, $\hat{x}(t_1^+)$ and $P(t_1^+)$ are employed as initial conditions for the next time step, and Equations (4.3) and (4.4.) are integrated from t_1 to t_2 to produce $\hat{x}(t_2^-)$ and $P(t_2^-)$. Equations (4.6-4.8), with t_2 and R_2 (instead of t_1 and R_1), are then employed to define $\hat{x}(t_2^+)$ and $P(t_2^+)$. The Kalman filter is recursive (as opposed to batch) because new concentration estimates are obtained each time a measurement is taken. Another property of the Kalman filter, which is very important in the determination of sampling strategies, is that if Equation (4.1) is linear in x or can be approximated by a linear function, then the variance equations (Equations (4.4), (4.7), and (4.8)) are independent of the actual measured concentrations $y(t_1),\ldots y(t_n)$ and depend only on the quality of the measurements, defined by $R_1,\ldots,R_n$. This allows the computation of the variance and an evaluation of the effectiveness of a sampling strategy before the sampling begins.

A SIMPLE KALMAN FILTER EXAMPLE

Probably the simplest mathematical model of the behavior of a pollutant in a lake is the scalar differential equation

$$\dot{x} = -ax + u(t) + w(t) \tag{4.9}$$

where $x(t)$ = concentration of the pollutant at time t, $u(t)$ is the input rate to the lake (for example, an industrial discharge), a is the positive constant sinking or degradation rate, and $w(t)$ is the model error resulting from either imperfect understanding of the physical, chemical, or biological mechanisms that affect $x(t)$, uncertain values for a, or inadequate characterization of the loading or forcing functions, or any combination of these. Suppose that two measurements of x are to be made at t_1 and t_2 with errors $v(t_1)$ and $v(t_2)$ that have mean values of zero and variances R_1 and R_2.

To apply the Kalman filter, statistics associated with the mathematical model must also be supplied. Suppose that the period of interest begins at $t_0 < t_1$ with initial estimates of $\hat{x}_0$ and P_0 that are obtained either by measurement or by model propagation from a time prior to t_0. To illustrate the behavior of the Kalman filter, suppose that the model errors are constants with zero mean values and variances Q_1 and Q_2. Also, suppose that the forcing function, $u(t)$, has a constant value of u_1 between t_0 and t_1 and a value of u_2 between t_0 and t_1.

With these assumptions, the prediction equations between measurements corresponding to Equations (4.3) and (4.4) are

$$\dot{\hat{x}} = -a\hat{x} + u_i \tag{4.10}$$

$$\dot{P} = -2aP + Q_i, \tag{4.11}$$

which are easily integrated to form the solutions

$$\hat{x}(t) = \left[\hat{x}(t_i^+) - u_{i+1}/a\right]e^{-a(t-t_i)} + u_{i+1}/a \tag{4.12}$$

$$P(t) = \left[P(t_i^+) - Q_{i+1}/2a\right]e^{-2a(t-t_i)} + Q_{i+1}/2a \tag{4.13}$$

where $\hat{x}(t_0^+) = \hat{x}_0$ and $P(t_0^+) = P_0$. The values of $\hat{x}(t_1^+)$ and $P(t_1^+)$ after measurement are determined by Equations (4.6-4.8),

$$\hat{x}(t_1^+) = \hat{x}(t_1^-) + \left[K_1\, y(t_1) - \hat{x}(t_1^-)\right] \tag{4.14}$$

$$P(t_1^+) = (1-K_1)\, P(t_1^-) \tag{4.15}$$

$$K_1 = \frac{P(t_1^-)}{P(t_1^-) + R_1} \tag{4.16}$$

where, from Equations (4.12) and (4.13),

$$\hat{x}(t_1^-) = (\hat{x}_0 - u_1/a)e^{-a(t_1-t_0)} + u_1/a \tag{4.17}$$

$$P(t_1^-) = (P_0 - Q_1/2a)e^{-2a(t_1-t_0)} + Q_1/2a \tag{4.18}$$

For the sake of illustration, suppose that $y(t_1)$ is a very good measurement compared to the prediction (R_1 is much less than $P(t_1^-)$) and vice versa for the $y(t_2)$ measurement (R_2 is much greater then $P(t_2^-)$). Note that because the model differential equation is stable (that is, $-a < 0$), use of

the dynamic model improves the accuracy of the estimate if $P_o > Q_1/2a$ (see Figure 1).

Similar estimates can be developed at t_2 with the results shown in Figure 1. In this case, Equation (4.16) implies $K_1 \approx 1$ (because R_1 is much less than $P(t_1^-)$) and $K_2 \approx 0$ (because R_2 is much greater than $P(t_2^-)$).

SUMMARY

The Kalman filter equations for a scalar differential equation process model with discrete measurements have been presented, and a simple water quality example was employed to illustrate the behavior of the equations. The Kalman filter equations provide appropriate weighting to both imperfect model predictions and measurements to produce an overall best estimate of concentrations based on minimizing the variance at each step. If the model equations are linear or can be approximated by a linear system, then it is possible to propagate the variance of the concentration values as a function of the uncertainty of the measurements, model parameter values, model forcing functions, and model structure. However, the estimates of the error propagation are independent of the actual measurements themselves. The overall techniques of Kalman filtering are summarized in Figure 2. In the following sections, the Kalman filter equations will be used in the determination of optimal sampling strategies for total phosphorus and chlorides in Lake Michigan and phytoplankton and nutrient dynamics in Saginaw Bay.

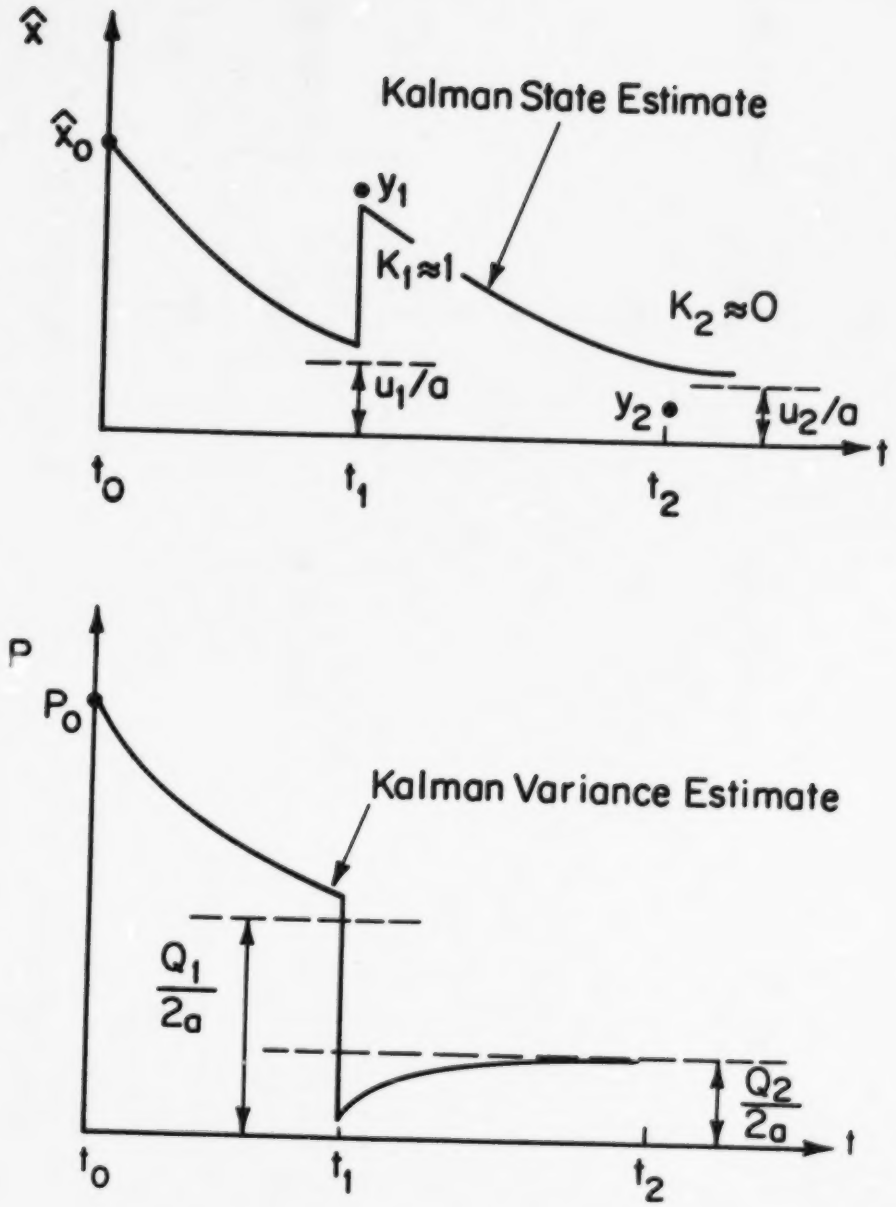

Figure 1. Changes in estimates of the state variable and variance according to Kalman filtering technique.

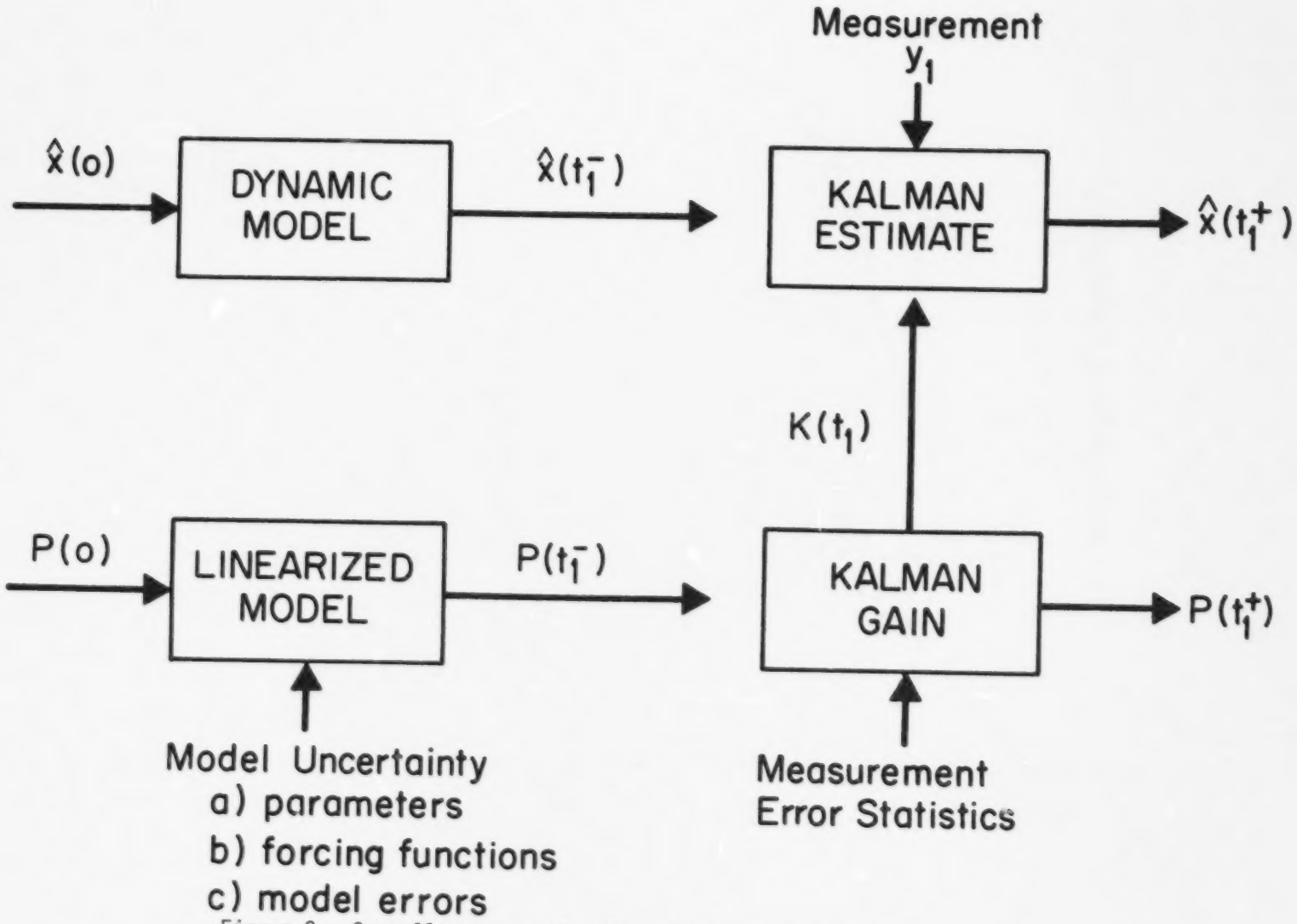

Figure 2. Overall summary of Kalman filter technique.

SECTION 5

AN APPLICATION TO LAKE MICHIGAN CHLORIDE AND TOTAL PHOSPHORUS TREND DETECTION

INTRODUCTION

One goal of the International Surveillance Program for the Great Lakes is to detect long-term changes in the concentrations of chloride ion and total phosphorus in each of the lakes. This section examines the cost-effectiveness of such a surveillance program for Lake Michigan and demonstrates how measurements of lake concentrations and mass balance models may be effectively employed together for trend detection. When appropriate, the extension of the techniques to other large lakes and water quality variables will be discussed.

The present surveillance plan for Lake Michigan involves lakewide sampling for two successive years every nine years and tributary sampling 26 times per year. Material balance models are not normally considered as sources of information that can be utilized, along with data, to estimate concentration changes and thereby detect trends. This research demonstrates how uncertain parameters in mass balance models of lakewide average concentrations can be interpreted as random variables, so that both the model and data can be employed in a Kalman filter. If the filter is used to estimate the accuracy of lakewide average concentrations over the next thirty years and a sampling program is prespecified, then the standard deviations associated with the accuracy of the estimates can be precomputed. The estimated errors must be small enough for trend detection, thus the standard deviations must satisfy upper bound constraints.

It is also shown that the problem of choosing the appropriate number of days for which tributaries must be sampled is equivalent to that of choosing a controllable model error covariance matrix. The minimum-cost lake surveillance and tributary sampling programs that meet accuracy criteria on the estimates of lakewide average concentrations are determined. The criteria are chosen to guarantee that trends will be detected with some specified statistical confidence. A series of measurement strategy optimization problems are solved to illustrate the role that Kalman filter techniques can play in the design of monitoring programs.

DERIVATION OF THE STOCHASTIC MODEL

The Indicator of Trend

Chloride is a conservative pollutant that occurs primarily in dissolved form and is affected little by the annual biological cycle. Total phosphorus, however, includes phosphorus that is utilized in the biochemical cycle of phytoplankton and other organisms. As phytoplankton cells mature and die, they accumulate at the sediment-water interface, resulting in removal of phosphorus from the water column. A measure of the phosphorus available for biological production during a particular year is provided by the lakewide average concentration of total phosphorus following spring overturn. Because ice at this time may prevent a sampling program from being implemented, it is convenient to assign May as the month when chloride and total phosphorus concentrations are relevant to trend detection.

The lakewide average concentrations of chloride and total phosphorus for May of year n are defined, respectively, by

$$X_1(n) = m_1(n)/V(n) \text{ and } X_2(n) = m_2(n)/V(n) \qquad (5.1)$$

where $m_1(n)$ and $m_2(n)$ are the pollutant masses in the lake (including the nearshore zone but excluding the sediments) and where $V(n)$ is the lake volume. Lakewide average concentrations may be crude indicators of trend if severe concentration gradients exist. However, if the lake is segmented spatially, then mass balance models must be derived for each segment average, and the resultant model must include uncertain parameters for advective and dispersive mass transfer.

In order to derive difference equations for the lakewide average concentrations, equations are first determined for the masses $m_1(n)$ and $m_2(n)$. During year n (May of year n to April of year n+1), mass exits the lake through the Straits of Mackinac (SM) and the Chicago Sanitary and Ship Canal (CSSC) and enters from tributary, atmospheric, and direct loading. Furthermore, a fraction of the total phosphorus that reaches the sediments during a year is incorporated into refractory deposits, resulting in a net sedimentation loss (Hutchinson, 1957). These sources and sinks are approximated on a net annual basis rather than on a seasonal basis, and their statistical characteristics are evaluated with information presently available.

Straits of Mackinac

The net annual flow through the SM is toward Lake Huron; however, at certain times of the year the flow is toward Lake Michigan. The net exchange of pollutant mass between the two lakes during one year is the difference between the flux towards Lake Michigan and the flux towards Lake Huron. Each flux is the product of an annual flow and an effective concentration. The effective concentration lies in the range of instantaneous concentrations during the year. If q_{in} and q_{out} are the components of annual flow toward and away from Lake Michigan, and if X_{in} and X_{out} are the effective concentrations on the Lake Huron and Lake Michigan sides of the SM, then the net loss from Lake Michigan is,

$$X_{out}\, q_{out} - X_{in}\, q_{in}. \tag{5.2}$$

If $X_{in} = X_{out}$, then the net loss is proportional to $q_{out} - q_{in}$, which is the net annual flow. However, chloride and total phosphorus concentrations in Lake Huron are less than those in Lake Michigan because of dilution by Lake Superior water. A conservative upper bound on the net loss is obtained by setting $X_{in} = 0$, in which case the loss is proportional to q_{out}. Therefore, the actual loss must lie between $X_{out}\,(q_{out} - q_{in})$ and $X_{out}\, q_{out}$ and is denoted by $X_{out}\, q_s$, where q_s is an uncertain effective outflow. Quinn (1976) has computed net annual flows, $q_{out} - q_{in}$, of 224 x $10^{11}\ell$ to 522 x $10^{11}\ell$. The validity of the technique has been upheld by current meter data from Saylor and Sloss (1976). Furthermore, Quinn suggests that these current meter data can be employed to obtain the following relationship between net flow and gross flow,

$$q_{out} \approx 1.67\ (q_{out} - q_{in}). \tag{5.3}$$

If Equation (5.3) is used to estimate the gross outflow for 1950-1966 from Quinn's net flow, then a range of 374 x $10^{11}\ell$ to 871 x $10^{11}\ell$ results.

The effective flow for each year, n, $q_s(n)$, is interpreted as a random variable, uniformly distributed between the minimum net flow and maximum gross flow for 1950-1966. The mean and standard deviation of this random variable are, respectively, 547 x $10^{11}\ell$ and 186 x $10^{11}\ell$. The effective concentration on the Lake Michigan side of the SM for year n, $X_{out}(n)$, must lie in the range of concentrations in the outflowing water during the year. It is assumed that this range is narrower than the range of concentrations over the entire lake for May of year n. The effective concentration is represented as the sum of the lakewide average concentration in May, X(n), and a deviation, $\varepsilon_s(n)$. That is,

$$X_{out}(n) = X(n) + \varepsilon_s(n). \tag{5.4}$$

The deviation is a zero mean random variable that is representative of the spatial heterogeneity of the lake. Its standard deviation can be estimated from unpublished data collected in the northern half of the lake by the Great Lakes Research Division (GLRD) of the University of Michigan for April and June 1976. A statistical summary of the chloride data from thirty-seven stations sampled during the June cruise and similar results for total phosphorus for thirty-three stations sampled during the April cruise are provided in Table 1. Only stations of depth greater than twenty meters have been included to avoid bias resulting from nearshore pollution. For each station, the mean (unweighted with depth) and standard deviation of the data have been computed. The standard deviation of the station means is assumed to be representative of the variation in the data because the data suggest that the horizontal variation exceeds the vertical variation. These standard deviations are 0.32 mg Cl/ℓ and 1.6 μg P/ℓ. However, the total observed variation is a result of not only spatial heterogeneity, but also laboratory analysis error. Great Lakes Research Division has suggested that standard

TABLE 1. SUMMARY OF GLRD DATA

Chloride				Total phosphorus			
Station no.	Number of samples	Mean mg/ℓ	Standard deviation mg/ℓ	Station no.	Number of samples	Mean µg/ℓ	Standard deviation µg/ℓ
2	4	7.73	0.02	2	4	7.3	0.6
4	6	7.68	0.03	4	6	7.9	0.6
6	13	7.69	0.03	6	12	8.1	1.2
8	6	7.70	0.05	8	6	9.1	1.0
10	4	7.80	0.19	10	4	14.8	2.4
13	4	7.70	0.01	13	4	8.6	1.3
15	6	7.72	0.03	15	6	7.4	0.4
17	17	7.73	0.06	17	17	6.7	1.3
19	5	7.86	0.02	19	6	7.0	0.6
20	7	7.89	0.02	20	6	7.1	0.5
23	5	7.73	0.02	23	5	6.9	0.4
25	14	7.73	0.02	25	14	7.4	0.7
27	6	7.68	0.07	27	6	6.9	1.1
29	4	7.63	0.03	29	4	6.8	0.8
30	4	7.79	0.10	30	4	8.2	1.1
32	4	7.72	0.05	32	4	5.9	0.6
34	5	7.74	0.04	34	5	6.5	0.6
36	9	7.73	0.05	36	9	7.9	1.2
39	4	7.58	0.11	39	4	6.3	0.6
42	3	7.70	0.04	42	3	6.5	0.7
43	3	7.68	0.03	43	2	6.5	0.1
44	3	7.68	0.08	44	4	7.8	2.3
46	3	7.34	0.22	46	3	6.6	0.4
47	4	7.58	0.14	47	4	6.1	0.2
48	3	7.55	0.01	48	3	6.4	0.4
49	3	7.45	0.14	49	3	6.2	0.4
53	2	7.01	0.01	54	3	8.4	2.0
54	3	7.10	0.03	55	4	5.9	0.6
55	4	7.32	0.19	58	3	5.8	0.7
58	3	6.58	1.13	59	3	6.1	0.6
59	5	7.07	0.06	60	2	6.0	0.1
60	3	7.06	0.12	63	3	6.4	0.6
63	5	7.00	0.26	64	3	5.2	0.4
64	3	6.89	0.10				
67	6	7.84	0.06				
68	5	7.83	0.05				
69	3	7.90	0.06				
Mean of station means		7.55 mg/ℓ		Mean of station means		7.2 µg/ℓ	
Standard deviation of station means		0.32 mg/ℓ		Standard deviation of station means		1.6 µg/ℓ	

deviations for laboratory errors are 0.10 mg Cl/ℓ and 1.0 μg P/ℓ.[1] Therefore, the standard deviations for station concentrations about the lakewide average concentrations are 0.30 mg Cl/ℓ and 1.3 μg P/ℓ. These are employed for the standard deviations of $\varepsilon_{s_1}(n)$ and $\varepsilon_{s_2}(n)$, respectively, where subscripts have been introduced to distinguish chloride from total phosphorus.

The net losses of pollutant masses through the SM are, respectively,

$$\left[X_1(n) + \varepsilon_{s_1}(n)\right] q_s(n) \text{ and } \left[X_2(n) + \varepsilon_{s_2}(n)\right] q_s(n) \tag{5.5}$$

Chicago Sanitary and Ship Canal

The annual diversion of water from Lake Michigan to the Illinois River through the CSSC has been limited to 28.7×10^{11} ℓ since 1970 by U.S. Supreme Court decree. The outflow, denoted by $\bar{q}_c$, is interpreted as a known constant at this maximum value. The effective concentration in the outflow is interpreted in the same manner as for the SM with resulting losses of

$$\left[X_1(n) + \varepsilon_{c_1}(n)\right] \bar{q}_c \text{ and } \left[X_2(n) + \varepsilon_{c_2}(n)\right] \bar{q}_c \ . \tag{5.6}$$

The zero mean random variables, $\varepsilon_{c1}(n)$ and $\varepsilon_{c2}(n)$, are different random variables than $\varepsilon_{s1}(n)$ and $\varepsilon_{s2}(n)$ but have the same standard deviations, that is, 0.30 mg Cl/ℓ and 1.3 μg P/ℓ.

Refractory Sediment Deposits

For a lake in which the lakewide average phosphorus concentration in the spring is at steady state, the phosphorus retention coefficient is

$$R_p = (m_{in} - m_{out})/m_{in} \tag{5.7}$$

where m_{in} and m_{out} are the mass loading and mass outfall during a year. The apparent phosphorus settling velocity S[m/yr] is that velocity such that the net sediment loss for a year is $Sm/\bar{h}$, where m is the lakewide mass in the spring and $\bar{h}$ is the mean depth. According to Chapra (1975), the apparent settling velocity can be related to the retention coefficient by

$$S = R_p(q/A)/(1-R_p), \tag{5.8}$$

where q is the total outflow and A is the lake surface area. Although R_p is difficult to measure for Lake Michigan, data have been compiled for smaller lakes. Resultant apparent settling velocities, computed with Equation (5.8), are summarized in Table 2. These data suggest a range of 0.7 to 37.9 m/yr.

[1]Personal communication, Curtiss Davis, GLRD.

TABLE 2. APPARENT SETTLING VELOCITY FOR SMALL LAKES

Lake	S[m/yr]	Lake	S[m/yr]
[1]Four Mile	11.0,11.0	[3]Mendota	11.1
Raven	11.3,13.3		
Talbot	9.3	[4]Joseph	8.8
Bob	16.2,16.3	Rousseau	13.6
Twelve Mile + Boshkung	22.9,21.4		
Halls	25.5,29.4	[5]Conesus	35.8
Beech	8.6,16.8	Canadice	30.9
Pine	5.0,1.4	Honeoye	23.3
Eagle + Haliburton	8.6,14.6		
Oblong + Haliburton	14.5	[6]Washington	27.0
Rawaon	5.6,4.9,6.0		
Clear	4.3	[7]Leman	3.2
		Bay of Naples	14.1
[2]Brewer	3.7	Canadaligua	5.1
Clarke	17.0	Carlos	4.5
Costello	8.7	Carry Falls	20.2
Kearney	6.5	Cass	15.1
Aegerisse	12.1	Charlevoix	8.9
Bodensee	37.9	Higgins	2.1
Turlersee	26.0	Houghton	1.6
Zurichsee	11.3	Long (Aroostook Co.)	5.3
Hallwilersee	4.1	Long (Cumberland Co.)	8.6
Griefensee	15.3	Mattawamkegg	14.4
Pfaffikersee	23.1	Moosehead	4.6
Baldeggersee	11.8	Pelican	0.7
Tahoe	5.7	Rangeley	4.9
Found	7.2	Sebago	7.8
Little McCauley	8.8	Winnipesaukee	11.0

[1]Kirchner and Dillon (1975).

[2]Dillon and Kirchner (1975).

[3]Sonzogni (174).

[4]Michalski et al. (1973).

[5]Stewart and Markella (1974).

[6]Lorenzen et al. (1976).

[7]Larsen and Mercier (1976).

Multiple values represent different data sets.

The mechanisms that govern the formation of refractory deposits are complex. The exchange between the sediments and the overlying waters of a lake depends on currents and degree of stratification, on phytoplankton species composition, and on biochemical cycles at the interface. Harrison et al. (1972), for example, discuss the effect of oxygen and bacteria on the exchange. It would be extremely difficult to relate exchange mechanisms in Lake Michigan with those of the lakes in Table 2. Therefore, S will be interpreted as a random variable, uniformly distributed between 0.7 and 37.9 m/yr. The mean and standard deviation are, respectively, 19.3 and 10.7 m/yr. If $\bar{h}(n)$ is the mean depth of Lake Michigan, then the net loss of phosphorus to the sediments during the year n is

$$S(n)\, m_2(n)/\bar{h}(n). \tag{5.9}$$

Tributary Loads

The GLWQB has identified twenty-seven major tributaries in the Lake Michigan drainage basin. The mass of pollutant discharged into the lake during a year by a tributary is the integral of the instantaneous flux over the year. The Mean Value Theorem permits the integral to be replaced by a sum

$$\text{Load} = \sum_{d=1}^{365} X_d\, q_d \tag{5.10}$$

where q_d is the tributary discharge at the mouth during day d and X_d is an effective concentration of pollutant in the discharge at the mouth.

Although daily discharges are available for the tributaries from the U.S. Geological Survey Water Supply Papers, concentration measurements are normally taken only at monthly intervals. An estimate of the annual load for a tributary, based on a complete and accurate record of discharge but an incomplete and inaccurate record of concentration, may be obtained in the following manner. Assume that a concentration measurement is available for each day d in a set of D days and that this measurement serves as an estimate for X_d. Furthermore, assume that a concentration measurement is not made on each of the other 365-D days in set D' and the X_d, in this case, is estimated from past data on the tributary (for example, from a regression relationship between concentration and discharge).

The concentration estimate for a day in D may include error resulting from laboratory analysis, variation over the day, variation over the river cross section, and distance of the sampling station from the river mouth. The error is interpreted as a random variable with zero mean and standard deviation $\sigma_1 = 5.0$ mg/ℓ for chloride and $\sigma_2 = 50$ µg/ℓ for total phosphorus. The standard deviations were chosen as ten percent of typical concentrations of 50 mg Cl/ℓ and 500 µg P/ℓ. The concentration estimation error for a day in D' depends upon the availability of past data and upon the ability to employ these data and the known discharge to estimate the concentration X_d.

The error associated with this procedure is interpreted as a zero mean random variable whose standard deviation is equal to that of data available for the Maumee River (U.S. Army Corps of Engineers, 1975). The standard deviations of these data are 15.6 mg Cl/ℓ and 271 μg P/ℓ. These deviations are probably conservative upper bounds on the standard deviations of error associated with estimates of Lake Michigan tributary concentrations. This report does not consider tributary-specific standard deviations, but rather employs $\sigma_1' = 15.6$ mg Cl/ℓ and $\sigma_2' = 2.71$ μg P/ℓ for each tributary.

The error variances for the annual tributary loads are given by

$$\sigma_1^2 \sum_{D} q_d^2 + \sigma_1'^2 \sum_{D'} q_d^2 \quad \text{and}$$

$$\sigma_2^2 \sum_{D} q_d^2 + \sigma_2'^2 \sum_{D'} q_d^2 \,, \tag{5.11}$$

for chloride and total phosphorus. The calculations in Equation (5.11) require the tributary discharges q_d. In order to compute optimal lake measurement strategies for the next thirty years, however, standard deviations must be available now. Therefore, the q_d are replaced by the maximum daily discharge on record for the tributary. This discharge for the j^{th} tributary is denoted by $qmax^j$, and is computed from the maximum discharge at the closest station to the mouth of the tributary by correcting for ungauged drainage.

Conservative error variances for the total tributary loads for year n are then computed by

$$\left[\sigma_1^2 D(n) + \sigma_1'^2 (365-D(n))\right] \sum_{j=1}^{27} (qmax^j)^2$$

$$\left[\sigma_2^2 D(n) + \sigma_2'^2 (365-D(n))\right] \sum_{j=1}^{27} (qmax^j)^2 \tag{5.12}$$

where it is assumed that both chloride and total phosphorus are analyzed in the water samples collected on days D. The most appropriate number of days of sampling for year n, D(n), is interpreted as a variable to be determined in association with measurement strategy optimization.

Atmospheric Loads

Precipitation samples collected by Junge and Werby (1958) suggests that the annual chloride atmospheric load for Lake Michigan is between 6.4×10^{12} and 8.7×10^{12} mg. In the mass balance model, the chloride load is denoted

by the random variable $a_1(n)$, which is uniformly distributed between these extremes and, therefore has a mean of 7.6×10^{12} mg and a standard deviation 0.7×10^{12} mg. Murphy and Doskey (1975) collected precipitation samples from the shores of the lake. Their data are employed to compute a range of 12×10^{14} to 18.5×10^{14} µg for the annual total phosphorus atmospheric load. This load is interpreted as a random variable, $a_2(n)$, uniformly distributed between the extremes, and thus has a mean of 15.3×10^{14} µg and a standard deviation of 1.9×10^{14} µg. If data become available that define more significant phosphorus loading, then the optimal strategies reported in this report should be recomputed.

Direct Loads

Pollutants from some industries and municipalities discharge directly to Lake Michigan or discharge to a tributary below the sampling point for that tributary. The U.S. Environmental Protection Agency (1972) has computed a direct annual phosphorus load for 1971 of 17×10^{14} µg, which is significant compared with the sum of 1970 tributary and direct loads of 97×10^{14} µg (Chapra, 1977). Corresponding data for the direct chloride loads are not available, although the sum of 1960 tributary and direct loads was computed by O'Connor and Mueller (1970). The direct loads are denoted by $\bar{d}_1(n)$ and $\bar{d}_2(n)$ and are interpreted as known constants because their standard deviations are probably small compared to those of the tributary and atmospheric loads.

Summary of the Model

The approximations for the sources and sinks of chloride and total phosphorus are employed to derive the stochastic difference equations for the lakewide masses:

$$m_1(n+1) = m_1(n) - \left[X_1(n) + \varepsilon_{s_1}(n)\right] q_s(n) - \left[X_1(n) + \varepsilon_{c_1}(n)\right] \bar{q}_c + \left[t_1(n) + a_1(n) + \bar{d}_1(n)\right]$$

$$m_2(n+1) = m_2(n) - \left[X_2(n) + \varepsilon_{s_2}(n)\right] q_s(n) - \left[X_2(n) + \varepsilon_{c_2}(n)\right] \bar{q}_c - S(n)\, m_2(n)/\bar{h}(n) + \left[t_2(n) + a_2(n) + \bar{d}_2(n)\right] \quad (5.13)$$

Quinn (1975) has computed Lake Michigan water levels for the first of May for 1900-1972. The levels have a standard deviation of 1.1 feet and can be converted to volumes with an accuracy of $\pm$ 0.4 percent.[1] Volumes range

[1]Personal communication, Leonard Schutze, U.S. Army Corps of Engineers.

from $4.89 \times 10^{15}\ell$ to $4.97 \times 10^{15}\ell$. Therefore, the volume has been interpreted as a constant, $\bar{V} = 4.93 \times 10^{15}$. Similarly, the average depth is $\bar{h} = 85$m. Therefore, the equations for lakewide average concentrations are

$$\begin{aligned} X_1(n+1) &= \left[1 - \bar{q}_s/\bar{V} - \bar{q}_c/\bar{V}\right] X_1(n) \\ &\quad - \frac{1}{\bar{V}} \left[\bar{q}_s\, \varepsilon_{s_1}(n) + \bar{q}_c\, \varepsilon_{c_1}(n) + X_1(n)\, \tilde{q}_s(n)\right] \\ &\quad + \frac{1}{\bar{V}} \left[t_1(n) + a_1(n) + \bar{d}_1(n)\right] \\ X_2(n+1) &= \left[1 - \bar{q}_s/\bar{V} - \bar{q}_c/\bar{V} - S(n)/\bar{h}\right] X_2(n) \\ &\quad - \frac{1}{\bar{V}} \left[\bar{q}_s\, \varepsilon_{s_2}(n) + \bar{q}_c\, \varepsilon_{c_2}(n) + X_2(n)\, \tilde{q}_s(n)\right] \\ &\quad + \frac{1}{\bar{V}} \left[t_2(n) + a_2(n) + \bar{d}_2(n)\right] \end{aligned} \tag{5.14}$$

where $\tilde{q}_s(n) = q_s(n) - \bar{q}_s$ and $\bar{q}_s$ is the mean of $q_s(n)$. The terms $\varepsilon_{s_1}(n)\tilde{q}_s(n)$ and $\varepsilon_{s_2}(n)\tilde{q}_s(n)$ are small and have been neglected.

The apparent annual phosphorus loss rate may be interpreted as a model state ($X_3 = S/\bar{h}$) with trivial dynamics

$$X_3(n+1) = X_3(n) \tag{5.15}$$

and a random initial condition. Of course, by writing Equation (5.15), it is hypothesized that the apparent loss rate is constant in time with some uncertain value. Although this may be strictly incorrect, it is desirable to demonstrate that the estimate of an uncertain model parameter can be improved, that is, its error variance reduced by interpreting the parameter as a model state. With this interpretation, Equations (5.14) and (5.15) represent a three-dimensional nonlinear stochastic model with states X_1, X_2, and X_3.

At the initial year, n = 1976, the three state variables are uncertain. From GLRD data in Table 1, mean values of 7.55 mg Cl/ℓ and 7.2 μg P/ℓ are computed for X_1 (1976) and X_2 (1976), respectively. The accuracy of these estimates depends on the variance of point concentrations in the lake and on the number of samples employed in the computation of the means. If the average of L(n) station concentrations serves as the measurement, then it is possible to determine a formula that can be used to relate the measurement error and L(n) (DePalma, 1977). If δ^2 is the variance resulting from the

heterogeneous nature of the lake and γ^2 is the variance resulting from laboratory analysis error, then the overall measurement error variance is

$$(\delta^2 + \gamma^2)/L(n). \tag{5.16}$$

The overall error variance of a measurement and Equation (5.16) are used to compute the standard error of the initial concentration estimates. The standard errors are 0.05 mg Cl/ℓ and 0.29 μg P/ℓ using data in Table 1.

An estimate for S in 1976 is 19.3 m/yr from Table 2. The standard deviation of the error in this initial estimate is the standard deviation associated with the uniform distribution, that is, 10.7 m/yr. Note that this does not equal the standard deviation of the data in Table 2 because these data were only employed to establish a range for S. A summary of the model parameters, constants, and initial states in given in Table 3.

Kalman filter State Estimation

Equations (5.13), (5.14), and (5.15) constitute a nonlinear stochastic model with uncertain states (X_1, X_2, and X_3), uncertain parameters (ε_{s1}, ε_{s2}, ε_{c1}, ε_{c2}, $\tilde{q}_s$, a_1, a_2, t_1, and t_2), and known constants ($\bar{q}_s$, $\bar{q}_c$, $\bar{V}$, $\bar{d}_1$, and $\bar{d}_2$). The Kalman filter (Sage and Melsa, 1971) is a method that can be used to calculate an unbiased minimum variance estimate of the state variables (chloride and total phosphorus). A detailed description of the basis and approach of the Kalman filter is described in Appendix A. Briefly, the method requires statistical characterization of both the model equations and the measurements but does not depend on the actual measurements themselves. It is this property of the filter that allows the development of an a priori optimal measurement strategy. If estimates of the state variables are also desired, then measurements are required. In order to implement the linearized Kalman filter, the nonlinear state equations are linearized about nominal states that are computed by setting each uncertain parameter and initial state to its mean value and then solving the state equations (Equations (5.13), (5.14), and (5.15)). The nominal states have been computed assuming that future loads are the same as present loads; however, the Kalman filter approach is also applicable if future loads can be represented as known functions of time.

The Kalman filter combines the model and measurements to compute an estimate of the lakewide average concentration, which is theoretically more accurate than estimates based on the model or measurements alone. The estimation error variance, which is a measure of the accuracy of the Kalman estimate, can be computed, and it depends on the model parameter variances and measurement error variance but not on the actual measurements. Once the number of days, D(n), on which tributary samples are collected and the number of stations, L(n), at which lake samples are collected have been specified (for a number of years beyond 1976), the estimation error variances can be computed. Furthermore, D(n) and L(n) may be chosen to meet constraints imposed on the estimation error variances.

TABLE 3. A SUMMARY OF PARAMETERS, CONSTANTS, AND INITIAL STATES

Uncertain parameter	Description	Mean	Standard deviation	Unit
ε_{s_1}, ε_{s_2}	Deviation of SM concentration from lakewide average	0	0.30	mg/ℓ
		0	1.3	µg/ℓ
ε_{c_1}, ε_{c_2}	Deviation of CSSC concentration from lakewide average	0	0.30	mg/ℓ
		0	1.3	µg/ℓ
$\tilde{q}_s$	Deviation of SM effective flow from mean $\bar{q}_s$	0	186×10^{11}	
$t_1 + \bar{d}_1$, $t_2 + \bar{d}_2$	Sum of tributary load and direct load[1]	934×10^{12}	$22\text{-}67 \times 10^{12}$	mg
		9.67×10^{14}	$2.2\text{-}11.6 \times 10^{14}$	µg
a_1, a_2	Atmospheric loads2	7.6×10^{12}	0.7×10^{12}	mg
		15.3×10^{14}	1.9×10^{14}	µg

(Continued)

[1]The means are for 1960 (chloride and 1970 (phosphorus). The range of standard deviations corresponds to $365 \geq D \geq 12$.

[2]The means are for 1955 (chloride) and 1974 (phosphorus).

TABLE 3. (Continued)

Constant		Value	Unit
$\bar{q}_s$	Mean effective flow through SM	547×10^{11}	ℓ
$\bar{q}_c$	Flow through CSSC	28.7×10^{11}	ℓ
$\bar{V}$	Volume	4.93×10^{15}	ℓ
$\bar{h}$	Depth	85.0	m

Initial state	Description	Mean	Standard deviation	Unit
$X_1(1976)$	Chloride lakewide average concentration	7.55	0.05	mg/ℓ
$X_2(1976)$	Phosphorus lakewide average concentration	7.2	0.29	µg/ℓ
$X_3(1976)$	Phosphorus loss rate $S/\bar{h}$	0.227	0.126	yr-1

DESIGN OF MEASUREMENT STRATEGIES

The Great Lakes Water Quality Board (GLWQB) (1976) has recommended a long-term schedule for intensive sampling of the off-shore waters of Lake Michigan. The lake will be sampled two successive years every seven years (1976, 1977, 1985, 1986 ...). Tributaries will be sampled 26 times per year. One goal of the program is to detect trends in the concentrations of chloride and total phosphorus. This goal would be accomplished by comparing estimates of lakewide average concentrations for the years when samples are collected. The estimates of concentration for any one year would be based only on data from that year. No procedure is presently available for introducing mass balance information into the estimation process.

It is appropriate to first examine the effectiveness of the proposed GLWQB sampling program for the case where no mass balance information is utilized and the data are not processed by a Kalman filter. Consider a sampling program in which sixty deep-water stations are sampled two consecutive years every seven years. If it is assumed that four depth samples are collected at each station and are averaged to compute the station concentration and the mean of the station concentrations is interpreted as a measurement of the lakewide average concentration, then from Equation (5.16) the standard deviations of the chloride and phosphorus measurement errors are 0.04 mg/ℓ and 0.2 μg/ℓ, respectively.

In order to evaluate the effectiveness of this surveillance program, criteria for trend detection must be established. For demonstration purposes, it will be assumed that changes of 1.0 mg Cl/ℓ and 1.0 μg P/ℓ must be detected with 0.90 probability. Measurement errors must, therefore, fall below 0.5 mg Cl/ℓ and 0.5 μg P/ℓ with 0.90 probability. In order to convert these criteria into constraints on the measurement error variances, it could be assumed that measurement errors are normal random variables (which is not true in general) or the Chebyschev Inequality (Davenport, 1970) could be used that applies to any random variable regardless of its density function. To avoid any unnecessary assumptions, the latter approach is chosen. This inequality guarantees, with a probability of p, that the estimation error will not exceed Δ, if the standard deviation does not exceed $\Delta\sqrt{1-p}$. Therefore, (for $p = 0.90$ and $\Delta = 0.5$) the constraints on the standard deviations are 0.158 mg Cl/ℓ and 0.158 μg P/ℓ.

It is concluded that the GLWQB planned surveillance program does not include enough stations to meet the detection criterion for phosphorus ($0.2 > 0.158$ μg/ℓ), but includes more than enough stations to meet the criterion for chloride ($0.04 < 0.158$ mg/ℓ). Note that the measurement error variance will be the same for 1977, 1985, 1986, 1994, 1995, 2003, and 2004 if sixty stations are sampled each year and the Kalman filter is not employed to process the data. In order to meet the detection criteria (without the Kalman filter) a minimum of about 108 stations must be sampled according to Equation (5.16) (Strategy I).

Although the criterion for total phosphorus trend detection is not met by the monitoring program proposed by the GLWQB, a strategy may exist that satisfies the criterion but costs less than Strategy I. An interactive

optimization algorithm involving the solution of a sequence of linear programming problems (DePalma, 1977) has been applied to compute the minimum-cost strategy that satisfies the chloride and total phosphorus detection criterion every nine years (Strategy II). The number of lake stations L(n) is chosen between zero and 168, the latter corresponding to two ships, operating two weeks, each sampling six stations per day. The number of days of tributary sampling D(n) is chosen between twelve and 365. The optimal strategy is summarized in Table 4. Tributary samples, beyond the basic twelve per year, are not requested by the strategy, and lakewide sampling is only requested for those years when constraints have been imposed on the standard deviations. The standard deviations corresponding to Strategy II and all other strategies to be discussed in this chapter have the following basic characteristics. The chloride standard deviations are well below imposed constraints of 0.158 mg/ℓ for all thirty years, and the phosphorus standard deviations equal the constraint of 0.158 µg/ℓ for the years when a constraint is imposed and exceed 0.158 µg/ℓ for all other years. Clearly, requirements for phosphorus detection control the measurement strategy and the optimal strategy would not change if chloride were ignored in the optimization.

Employment of the Kalman filter has reduced the cost required for trend detection. If four water samples are collected at a station and analyzed for all basic chemicals, including chloride and total phosphorus, then the total cost incurred per transect is $3,320. If one water sample is collected from each tributary and analyzed for all basic chemistry, then the total cost incurred in sampling the system is $3,300 per day.[1] Only twelve days of tributary sampling are requested by the optimal strategy, which represents a saving of $46,200 each year, and lake samples are requested only for those years when constraints are imposed. The number of lake stations required for each of the four years when a constraint is imposed is shown in Table 4 as Strategy II. If no model were employed (Strategy I), 108 stations are required each year resulting in a four-year cost of $239,000. The model permits a reduction in cost of lake sampling to $227,000. The overall savings for lake and tributary sampling is $1,398,000 over a thirty-year period.

Only $12,000 in lake sampling costs are saved by utilizing the mass balance model because the formulation of the standard deviation of the tributary load as a function of D(n) is very conservative (being based on maximum observed discharges and Maumee River concentration data). The above minimum-cost strategy has been recomputed under somewhat more realistic assumptions: that daily discharges equal the average daily discharge on record for a tributarty; that σ_1 and σ_2 are 1/50 of the values previously assumed; and the σ_1' and σ_2' assume the values originally assigned to σ_1 and σ_2. The number of lake stations requested by the optimal strategy (Strategy II) is presented in Table 5 and is substantially less than for the conservative assumptions. The costs for the more liberal ($153,000) and conservative ($227,000) cases bracket the cost that would be computed if actual values for the discharges and standard deviations were available today.

[1]Sampling costs provided by William Richardson, EPA, Grosse Ile.

TABLE 4. REQUIRED NUMBER OF SAMPLING STATIONS AND COSTS FOR CONSERVATIVE FORMULATION OF TRIBUTARY LOAD ERROR

Strategy	Year				Cost [$]
	1977	1986	1995	2004	
I	108	108	108	108	1,625,000
II	106	108	100	97	227,000
III	106	108	100	97	227,000
IV	106	108	100	96	227,000
V	92	107	100	96	218,000
VI	84	95	94	93	201,000
VII	83	91	91	91	196,000
VIII	76	78	72	69	162,000
IX	67	68	63	61	142,000
X	88	90	82	79	187,000
XI	70	72	65	61	148,000
XII	52	54	46	43	107,000
XIII	34	36	29	26	68,000
XIV	25	27	21	18	49,000

TABLE 5. REQUIRED NUMBER OF SAMPLING STATIONS AND COST FOR MORE REALISTIC FORMULATION OF TRIBUTARY LOAD ERROR

Strategy	Year				Cost [$]
	1977	1986	1995	2004	
I	108	108	108	108	1,625,000
II	106	107	45	19	153,000
III	106	107	41	14	147,000
IV	106	107	33	10	141,000
V	84	106	45	19	139,000
VI	56	64	36	16	94,000
VII	55	0	0	0	30,000
VIII	76	77	33	14	110,000
IX	67	68	29	13	96,000
X	88	89	36	14	125,000
XI	70	72	27	10	98,000
XII	51	53	18	6	70,000
XIII	33	36	11	3	45,000
XIV	25	27	8	2	33,000

It is of considerable interest to determine the reduction in measurement cost that can be realized by applying research funds to the study of the various mass balance model parameters. Inaccuracies in these parameters depend on uncertainty in the pollutant concentrations in outflowing water, uncertainty in the effective SM flow, uncertainty in atmospheric loads, and uncertainty in tributary loads. Reduction of uncertainty associated with the outflowing water would require the implementation of a routine sampling program and will not be considered here. The second component may be reduced by intensive current metering and sampling in the SM to identify the nature and magnitude of the return flow. Consider a hypothetical situation in which the effective flow at SM is known precisely. The minimum-cost measurement programs in Tables 4 and 5 (Strategies III) have been computed based on this hypothesis, with conservative and liberal assumptions for the formulation of tributary load error variance. The costs entered in these tables represent the minimum costs achievable under such a research program because the effective SM flow cannot be measured precisely. The difference between Strategies II and III must be weighed against the cost of the research.

A third component of the covariance matrix may be reduced by an intensive atmospheric-load sampling program. The program would not have to be routine because atmospheric loads would not be expected to change significantly over the next thirty years. Consider a hypothetical situation where the atmospheric loads are known precisely. The minimum-cost measurements in Table 4 and 5 (Strategies IV) have been computed and represent an additional reduction in cost compared to Strategies II. The savings must be weighed against the cost of collecting and analyzing precipitation and dustfall samples.

The fourth and final component of the covariance matrix, uncertainty in tributary loads, has been assumed to be controllable in this report. However, because of the high cost of sampling the tributary system, none of the strategies computed so far or to be computed, contain any samples beyond the routine twelve per year. This is true for both the conservative and liberal assumptions concerning the tributary load error variance as a function of the number of samples.

The apparent annual phosphorus loss rate, X_3, is also a model parameter but has been interpreted as a state variable in the stochastic model. This permits the linearized Kalman filter to estimate this rate in the same manner as it estimates chloride and phosphorus lakewide average concentrations. Of course, the estimate is not based on measurements of the rate itself but rather on measurements of the total phosphorus lakewide average concentration. The standard deviation of $X_3(n)$ is constant between measurements and decreases when a measurement is made. In general, the accuracy of the estimate can be significantly improved by the end of the thirty year sampling program. However, it would be desirable to dedicate enough research to the mechanisms of total phosphorus removal in Lake Michigan to reduce the present uncertainty in X_3. If mechanisms of sinking and removal could be correlated with apparent settling velocity, then the range of uncertainty in X_3 could be reduced from the present range of $\pm$ 19.6 m/yr. Minimum-cost measurement strategies in Tables 4 and 5 have been computed under hypotheses

that the range of S is reduced immediately to $\pm$ 5.0 m/yr (Strategy V), $\pm$ 1.0 m/yr (Strategy VI), or $\pm$ .5 m/yr (Strategy VII). It is evident that this improvement in model accuracy can provide a significant reduction in measurement cost. A decrease in the range of S beyond $\pm$ 5.0 m/yr, however may be difficult given the present understanding of phosphorus exchange mechanisms.

Next, consider the effect of total phosphorus laboratory analysis error on the optimal cost. The variance of laboratory analysis errors affects the error of a lakewide measurement in Equation (5.16) where δ^2 is the variance resulting from spatial heterogeneity and γ^2 is the variance resulting from laboratory error. Minimum-cost measurement (Strategy VIII) and (Strategy IX) in Tables 4 and 5 correspond to cases where the laboratory standard deviation is reduced from its present value of 1.0 µg P/ℓ to 0.5 µg P/ℓ and 0.1 µg P/ℓ. The reduction in measurement costs is significant but must be weighed against the research cost necessary to improve the present analysis technique. Note that the reduction in error is limited by the variation of point concentrations about the lakewide average concentration that cannot be altered.

Finally, reductions in the optimal cost can be achieved by relaxing the criterion of trend detection. Instead of requiring that changes of 1.0 mg Cl/ℓ and 1.0 µg P/ℓ be detected with 0.90 probability, detection with 0.88, 0.85, 0.80, 0.70, and 0.60 probability may be acceptable. The Chebyschev Inequality can be used to compute the constraints that must be imposed on the standard deviations of estimation errors in order to meet the detection criterion. If it is assumed that the estimation errors are normal, then, in order to meet the detection criterion with 0.90 probability, standard deviations would only have to be maintained below about 0.3 mg Cl/ℓ and 0.3 µg P/ℓ. This approximately corresponds to the constraint imposed by the Chebyschev Inequality for 0.60 probability. Minimum-cost Strategies X to XIV have been computed corresponding to probabilities of 0.88 to 0.60. The cost of detection at 0.60 probability is about one-fifth the cost of detection at 0.90 probability, and a sharp increase in cost is incurred as the probability increases from 0.80 to 0.90. Specification of trend-detection criterion will likely remain an ad hoc scientific decision. The purpose of the methodology applied in this section is to analyze the effect of particular uncertainties on the estimation process once detection criteria have been established.

The optimal measurement strategies discussed in this section and summarized in Tables 4 and 5 have been computed based on trend detection every nine years. In general, the Kalman filter approach for trend detection demonstrates its superiority over conventional procedures (no model, only data) more lucidly if detection is required every year. Consider the case in which liberal statistics are employed for tributary loads and all other statistics are as presented in Table 3. This case will, therefore, be analogous to Strategy II except error variance constraints will be imposed every year instead of every nine years. The optimal strategy and cost are summarized in Table 6. It is observed that the required number of stations is greatly reduced after the first few years of the program. If the Kalman filter were not employed, then 108 stations would have to be visited each

TABLE 6. OPTIMAL MEASUREMENT STRATEGY AND COST FOR DETECTION EVERY YEAR

n	Number of stations	n	Number of stations	n	Number of stations
1	106	11	12	21	3
2	89	12	10	22	3
3	70	13	9	23	3
4	54	14	8	24	2
5	42	15	7	25	2
6	33	16	6	26	2
7	27	17	5	27	2
8	22	18	4	28	1
9	18	19	4	29	1
10	15	20	3	30	1
Total Cost = $301,600					

year costing $1,793,000 over thirty years. The optimal cost is only $301,600 when the filter is employed.

SUMMARY

A nonlinar model has been derived that describes the long-term dynamics of chloride and phosphorus lakewide average concentrations in Lake Michigan. Statistics for each uncertain parameter in the model have been approximated from available data. The nonlinear model has been linearized about a nomimal, so that the linearized Kalman filter can be employed. Finally, the role of this model was explored for measurement strategy design.

The monitoring strategy proposed by GLWQB cannot detect changes of 1.0 μg P/ℓ at 0.90 probability with or without the Kalman filter. However, a minimum-cost strategy that meets the detection criterion every nine years has been computed. The optimal strategy contains limited tributary samples for both conservative and liberal formulations of the tributary load error variance. It is concluded that such samples are not a cost-effective source of information for detecting trends in lakewide average concentrations. It is also concluded that the phosphorus error variance constraint controls the number of lake stations required for trend detection because the chloride error variance satisfies the constraints and thereby has no effect on the optimal strategy. Furthermore, the optimal lake sampling strategy is very simple. Lake samples must be collected only for those years when the detection criterion must be satisfied.

An investigation was conducted to determine the sensitivity of the optimal cost to the statistics of the mass balance model parameters. It is concluded that the calculated cost is most sensitive to the variance in the apparent phosphorus settling velocity, not as sensitive to the accuracy of laboratory analyses, and rather insensitive to the accuracy of the effective SM flow and the atmospheric loads.

The actual design of a Lake Michigan surveillance program entails economic and practical considerations and would take into account other goals besides chloride and total phosphorus trend detection. The analyses presented here simply illustrate the manner in which Kalman filtering techniques can aid in defining and subsequently reducing the requirements of trend surveillance programs.

SECTION 6

AN APPLICATION TO ANNUAL PLANKTON AND NUTRIENT CYCLES IN SAGINAW BAY

INTRODUCTION

Section 5 described the use of Kalman filtering techniques to derive optimal measurement strategies for long-term trend detection of chloride and total phosphorus concentrations in Lake Michigan. The major goal of Section 6 is to conduct a brief preliminary investigation of the applicability of similar techniques to define efficient sampling strategies for phytoplankton, zooplankton, and nutrients such as nitrogen and phosphorus in Saginaw Bay. Annual rather than long-term dynamic cycles and interactions will be considered in an aquatic system where significant spatial gradients also exist.

The EPA Large Lakes Research Station at Grosse Ile has supported an intensive limnological monitoring program in the bay since 1973. Measurements from this program have been used to develop nutrient and plankton models for the system. These models have been used to predict phytoplankton levels in the bay following enactment of various schemes to control the level of phosphorus input loading. These calculations of phytoplankton levels are based on model equations and parameter estimates derived by comparing the model output with actual phytoplankton concentrations observed during 1974 and 1975. It is assumed in these calculations that independent laboratory and field data are not available to determine the model parameters. However, data in the literature are used to establish ranges for these parameters.

Several interesting and practical questions arise concerning the reliability of such procedures. For example, how good are the estimates of the predicted peak or average phytoplankton concentrations under the assumed conditions? It is known that uncertainties in the calculations are caused by imperfect knowledge of each model parameter and each state variable initial condition. It would be useful to know how well the model parameters and initial conditions must be known in order to calculate the peak phytoplankton concentration to within a known or specified degree of certainty. If it is impractical or impossible to quantify the model parameters and initial conditions sufficiently, it may be necessary to supplement model calculations for future conditions with measurements to obtain more accurate estimates of peak phytoplankton concentrations. In these cases it is necessary to determine the appropriate minimum number, frequency, and location of measurements.

Systematic and formal procedures have not previously been used to address and resolve these kinds of questions associated with plankton-nutrient models. However, the results in this section illustrate a promising approach to these issues using Kalman filtering techniques.

Another class of problems in Saginaw Bay concerns the design of cost efficient sampling programs that can be used to better define the value of model parameters and initial conditions. For example, suppose it is desired to calculate the peak phytoplankton concentrations within a specified tolerance using the model without supplemental data. Then, the techniques can be used to estimate the required certainty associated with the model parameters and initial conditions. This desire to determine the model parameters and initial conditions is best fulfilled by performing field measurements directly in the bay. It is of interest to determine cost efficient sampling schemes (number and frequency of samples) to accomplish these goals. This section introduces a methodology involving the use of Kalman filtering techniques that can be used to calculate suboptimal and, eventually, the least expensive sampling program.

SAGINAW BAY NUTRIENT-PLANKTON MODEL

Spatial and temporal variations of limnological variables in Saginaw Bay are determined by solving dynamic differential mass balance equations for each of five finite segments or cells as illustrated in Figure 3. This figure also shows the location of the Saginaw River, which is the major source of nutrients to the bay. The bay is coupled to Lake Huron by advective and dispersive hydraulic transport. The general flow pattern among various model segments is represented by arrows in Figure 3. The major biological and chemical kinetic reactions and forcing functions that affect the plankton and nutrient annual dynamics are illustrated in Figure 4. The dynamic behavior of the limnological state variables in each completely mixed finite segment of the bay is obtained by numerically integrating a system of ordinary differential equations of the form

$$V \frac{dc}{dt} = Ac + VR + W \qquad (6.1)$$

where V is an nxn diagonal matrix of volumes, c is an nxl vector of the state variables, A is an nxn matrix of advective and dispersive transport, R is an nxl vector of kinetic interactions, and W is an nxl vector of input forcing functions for c. For m interacting variables and n finite segments, a total of mxn equations must be solved. For this example, the state variables are phytoplankton (expressed as chlorophyll a), herbivorous zooplankton, carnivorous zooplankton, organic nitrogen, nitrate nitrogen, ammonia nitrogen, organic phosphorus, and reactive phosphorus.

A simulation model called LAKE-1 was developed by Thomann et al., (1975) to describe the dynamics of similar phytoplankton-zooplankton-nutrient interactions in Lake Ontario and the effects of nutrient loadings on those interactions. This model was subsequently applied to Saginaw Bay by

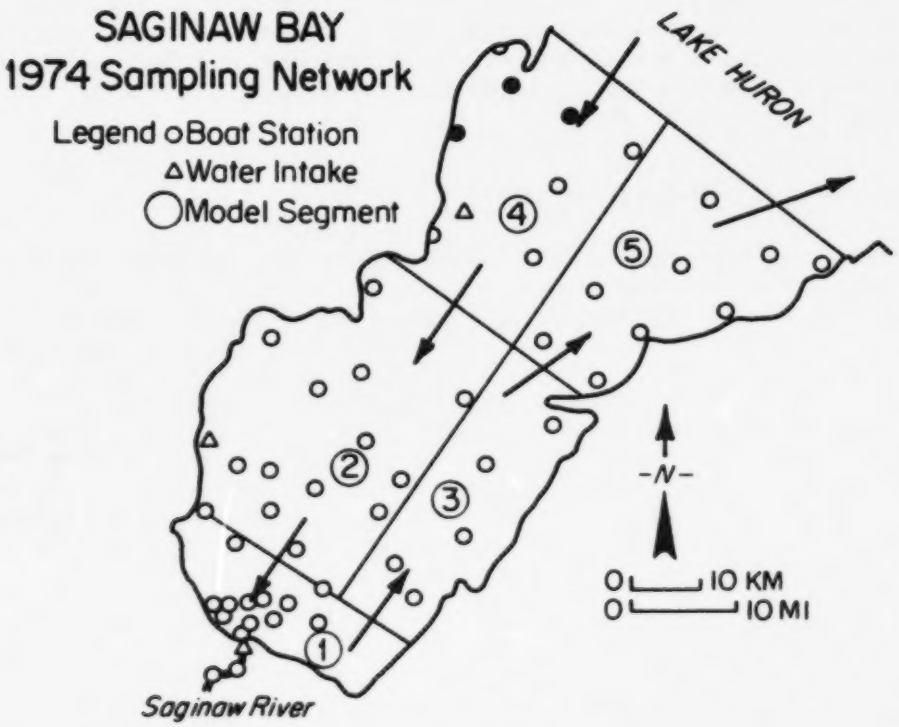

Figure 3. Saginaw Bay model segments, sampling stations, and flow pattern.

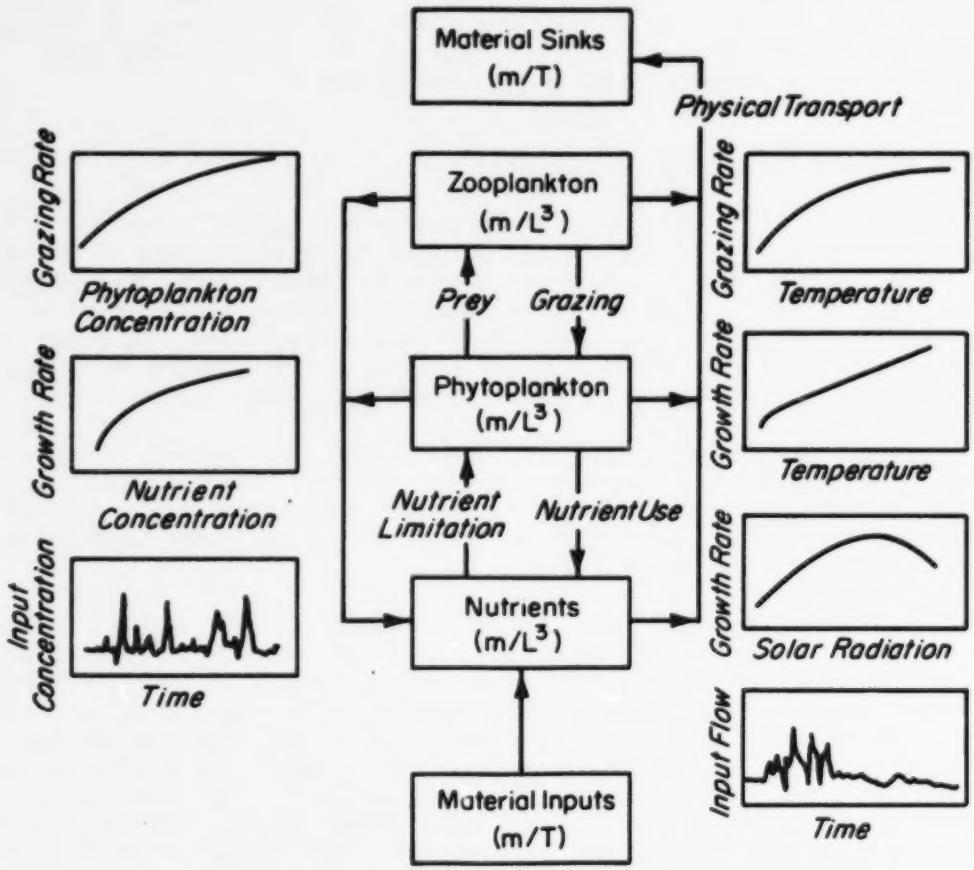

Figure 4. Saginaw Bay model biochemical reactions and forcing functions.

Richardson and Bierman (1976). The Richardson and Bierman model was adapted for this project to run on MTS (the University of Michigan Terminal System).

A general computer program was developed that implements models that can be described by a set of differential equations using an Adams predictor-corrector numerical integration method called DVDQ (Krogh, 1969). Solutions for a particular model are obtained by calling a subroutine that evaluates derivatives for the model using Equation (6.1) and any data files necessary to define time variable forcing functions. Temperature and light cycles are examples of time variable forcing functions used in the model. The equations for the derivatives and input data for this project were taken directly from a computer listing supplied by the EPA.

ERROR PROPAGATION WITHOUT MEASUREMENT

The theoretical development in Section 4 has suggested how the Kalman filter can be used to calculate the minimum-variance estimate of a state variable based on both a linear stochastic difference model for the system and actual field measurements. This section examines state variable error propagation for cases where measurements are not employed. Such applications might arise when the models are used to predict future water quality conditions that result from alternative nutrient control procedures.

Variance error propagation for linear systems is defined by Equation (4.4). This equation can be applied to nonlinear systems by constructing a linear system that defines the deviations of the states from a nominal solution generated from current best estimates of the parameters and state initial conditions (see Appendix A).

Estimates of the means and standard deviations for the model parameters are listed in Table 7. Standard deviations for the parameters were obtained by defining a range of values for a given parameter from the literature (Canale et al., 1976, Richardson and Bierman, 1976, Thomann et al., 1975) and assuming a uniform distribution over this range. For the purposes of this illustration and to limit computer costs, only seven parameters were chosen for study, while the other ten were assumed to be known perfectly (see Table 7). The initial values of the states are dependent on observed data and vary from model segment to segment. For the purposes of illustration, standard deviations associated with the states were arbitrarily equated to 0.25 times their mean value.

The computer generated nominal gives the time variable behavior of the states for each of the five model segments. These states depend on the model structure, parameter values, and forcing functions. The nominal states for model segment 5 are plotted in Figure 5. A 19-week time interval was used in the calculations to approximate the first phase of the phytoplankton growing season and to reduce computation costs. Time zero in this figure corresponds to a date of April 1. The calculated nominal states agree reasonably well with measured values of the states for all model cells and variables (Richardson and Bierman, 1976).

TABLE 7. ESTIMATED MEANS AND STANDARD DEVIATIONS FOR MODEL PARAMETERS

Parameters	Mean value	Standard deviation	Units
Nitrogen			
Half-saturation constant	0.025	0	mg/ℓ
Organic nitrogen decompositon rate	0.007	0	$day^{-1}deg^{-1}$
Ammonia to nitrate nitrification rate	0.015	0	$day^{-1}deg^{-1}$
Nitrogen-chlorophyll ratio	0.01	0.00175	mgN/μgCh
Phosphorus			
Half-saturation constant	0.005	0	mg/ℓ
Organic phosphorus decomposition rate	0.007	0	$day^{-1}deg^{-1}$
Phosphorus-chlorophyll ratio	0.00083	0.0003	mgP/μgCh
Zooplankton			
Conversion efficiency	0.06	0	
Endogenous respiration rate	0.0026	0.0011	$day^{-1}deg^{-1}$
Herbivorous and carnivorous zooplankton grazing rate	0.04	0.01	ℓ/mg C day deg
Phytoplankton			
Chlorophyll half-saturation constant	20	0	g/ℓ
Endogenous respiration rate (at 20)	0.0	0.0225	day^{-1}
Settling velocity	0.05	0	m/day
Saturated growth rate	0.20	0.091	day^{-1}
Optimum light intensity	350	0	langley/day
Carbon			
Carbon-chlorophyll ratio	0.025	0.02	mgC/μgCh

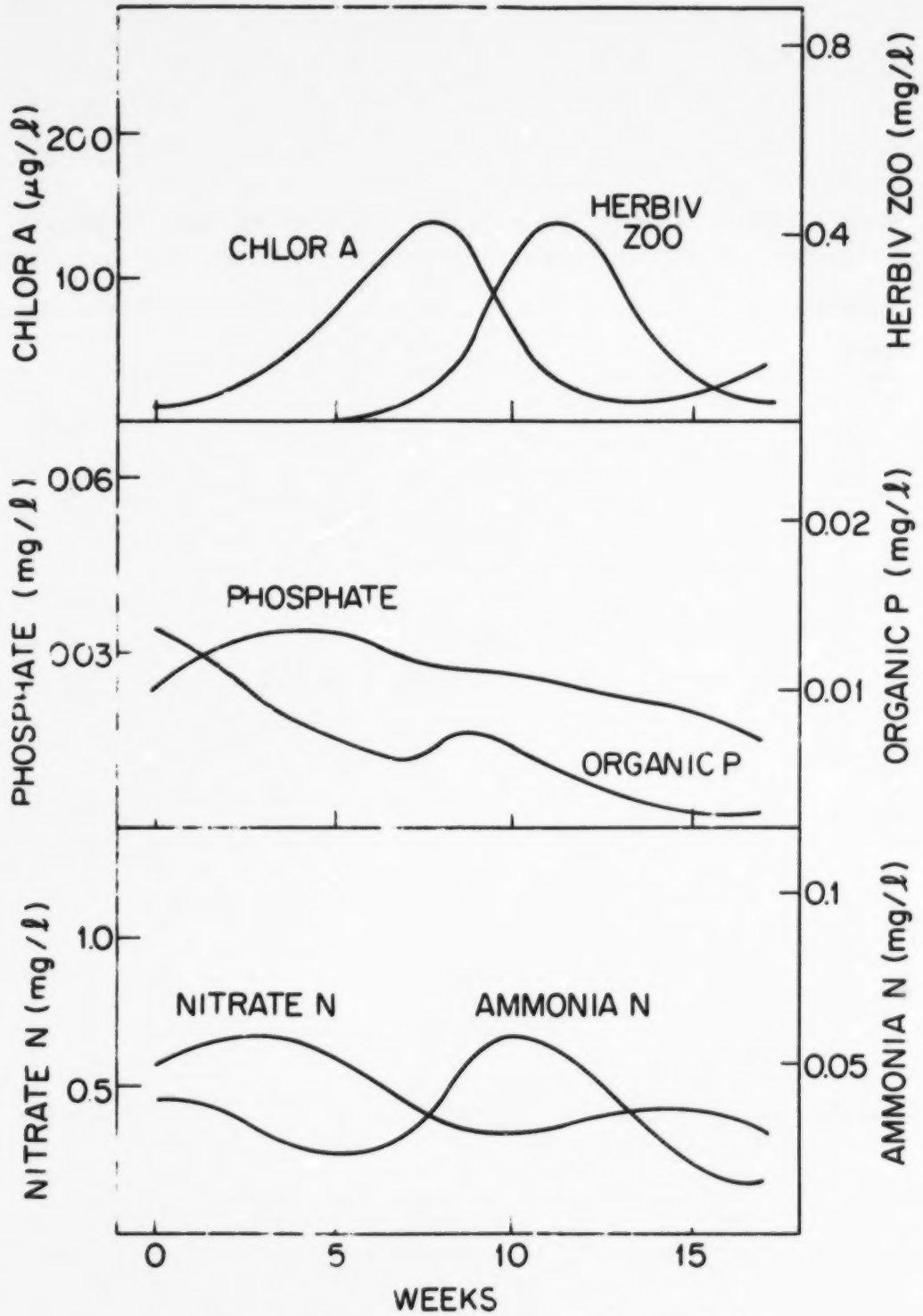

Figure 5. Nominal states for model segment 5.

Model application might require information regarding the uncertainty associated with a model caused by imperfect knowledge of the parameters and initial states, assuming that the model structure is exact in all other ways. These standard deviations have been computed according to Equation (4.4) assuming no measurements are made. Column (b) of Table 8 lists the calculated standard deviations at the peak values of chlorophyll a, herbivorous zooplankton, and carnivorous zooplankton using the data in Table 7 for the uncertainty in the seven selected parameters. Column (c) from this table lists the calculated standard deviations at the peak chlorophyll a and zooplankton levels for a case where the standard deviations for the seven selected parameters are reduced by a factor of ten. Column (d) gives similar calculations for the case where the original uncertainties are used for the seven parameters but the uncertainties associated with the initial states are reduced by a factor of ten. These results are an indication of the magnitude of error propagation that would result when an uncalibrated model is run using uncertain initial values, literature ranges for model parameters, and accurate forcing functions.

The results in Table 9 show that the largest calculated standard deviations occur in segment 1 for all three states. Therefore, according to these results, model predictions of the peak populations without measurements are the most unreliable in segment 1. Furthermore, the calculated standard deviations at the peaks in segment 1 are large compared to the mean value of the peak populations (see column a). This, of course, indicates that the model has limited value for predictions of peak states in segment 1 without measurements. Uncertainty accumulates as a function of time according to Equation (4.4), which for this case depends only on the nature of the system equations and parameter values. Relatively large errors occur in segment 1 because it has a small volume and depth, relatively warm temperatures, and high nutrient levels. On the other hand, the model has relatively good predictive capability for peak plankton levels in segment 5, which has a large volume and depth and low temperatures and nutrient levels.

The calculated standard deviations for the peak populations improve when the standard deviations associated with the seven parameters are reduced by a factor of ten. Such a reduction might be achieved by measurement of these parameters in laboratory or field experiments. The effectiveness of these improvements follows the flow pattern, which is in a counterclockwise direction. Standard deviations are only reduced about 1 percent in segment 4 whereas about 55 percent improvement is calculated for segment 5. An opposite phenomenon occurs when the uncertainty of the initial states is reduced and the uncertainty in the parameters remains the same. Reductions in the calculated standard deviations are most dramatic upstream in segment 4 (about 84 percent) and smaller in segment 5 (about 11 percent).

These calculated trends for the standard deviations of the states are consistent with physical considerations. Segments 4 and 2 are influenced more by boundary forcing functions and initial conditions and less by the structure of the equations and the model parameters. The changes in the states of segments 1, 3, and 5 are effected by input from adjacent model segments and the structure of the model and are relatively insensitive to the initial conditions.

TABLE 8. CALCULATED MEAN AND STANDARD DEVIATIONS AT THE PEAK POPULATIONS FOR ZERO MEASUREMENTS

Model States	Model cell no.	Time of peak (weeks)	(a) Mean value of state at the peak	(b) Standard deviation for normal values of parameters and initial states	(c) Standard deviation for improved parameters and normal initial states	(d) Standard deviation for improved initial states and normal parameters
Chlorophyll a	1	8	16.25	100.3	96.4	29.3
Herbivorous zooplankton	1	14	0.36	602.9	593.1	123.7
Carnivorous zooplankton	1	17	0.28	3,223.7	3,164.5	694.4
Chlorophyll a	2	9	8.52	69.3	68.1	14.3
Herbivorous zooplankton	2	14	0.24	155.3	152.8	31.9
Carnivorous zooplankton	2	17	0.10	261.5	257.2	54.2
Chlorophyll a	3	6	36.63	18.2	10.6	14.8
Herbivorous zooplankton	3	13	0.46	95.8	94.0	21.1
Carnivorous zooplankton	3	16	0.44	2,365.7	2,318.3	527.5
Chlorophyll a	4	10	4.52	47.2	46.8	7.63
Herbivorous zooplankton	4	15	0.17	50.6	49.9	10.09
Carnivorous zooplankton	4	17	0.14	13.7	13.5	2.86
Chlorophyll a	5	8	14.02	4.90	2.21	4.40
Herbivorous zooplankton	5	11	0.29	0.20	0.14	0.14
Carnivorous zooplankton	5	15	0.16	0.55	0.41	0.37

The results of these few simulations are provocative and raise several interesting questions. However, time and funding limitations and the original purpose of this section (to investigate the large-scale problem potential of the approach described in Section 4) did not permit additional analysis. For example, it would be important to study the effect of parameter identification with parameters other than the seven selected, to perform a more extensive study of the trade-off between more accurate knowledge of initial conditions as opposed to more accurate knowledge of parameters, and to perform Monte Carlo type simulations to determine the validity of Equation (4.4) in predicting standard deviations for this class of problems.

SUBOPTIMAL MEASUREMENT STRATEGY GENERATION

The previous section has examined the propagation of errors for the peak plankton populations when models alone were used to predict future conditions without supplemental measurements. Because the uncertainties associated with these predictions are unacceptably large, direct measurements and Kalman filtering techniques have been employed to reduce the error variance associated with the state variable estimates. A major goal of this section is to apply these techniques to a problem that is so large that automatic optimization as applied to trend detection in Lake Michigan (Section 5) is either too expensive or of questionable value because of limited statistical knowledge of the chemical and biological mechanisms.

The computer program that was utilized in Section 5 to determine optimal measurement strategies is a general purpose program (DePalma, 1977). The optimization algorithm in the program is very efficient for certain classes of problems, but it involves considerable storage. Automatic computation of full optimal sampling strategies for Saginaw Bay involves computer storage requirements well above the limit of the computing facilities at the University of Michigan. This difficulty can be addressed by modifying the approach to the problem to take advantage of the structure of the governing equations or by employing only the simulation portion of the program to analyze various measurement strategies. In this case, only the simulation portion of the program has been employed to demonstrate how reasonable suboptimal measurement strategies can be developed with a minimal amount of computation.

The mathematical model described earlier in this section is a nonlinear differential equation system involving eight state variables in each of five bay segments. Furthermore, it has been assumed that seven parameters in each segment have unknown values that are to be improved during the measurement process. Thus, seventy-five differential equations define the state model. Only the growing season ($t_j = 1,2,\ldots,19$) is considered for the range of admissible measurement times because of the large number of differential equations. The variance of a measurement can be improved by averaging a larger number of samples. However, practical considerations dictate that measurements at any time involve all eight state variables. In this section, the minimum measurement variance in a given week corresponds to a maximum practical sampling effort, while the maximum measurement variance corresponds to no measurement. The measurement strategy designer then

selects, with the aid of the Kalman filter, the set of weekly measurement variances, times, and segments that results in a cost-effective sampling program with acceptable accuracy.

The first step in this suboptimal measurement strategy selection process is the generation of the covariance matrix for the full measurement case (that is, minimum variance measurement for each week in each segment) which corresponds to a calibrated model with a full data set. Next, the covariance matrix is determined for the zero measurement case (that is, no measurements at any time) which corresponds to an uncalibrated model. These cases indicate the minimum and maximum variances attainable by the sampling program. The purpose of the optimal sampling strategy is to determine which partial data set will be adequate for accurate state estimation. Figures 6 to 9 show the nominal states and standard deviations for chlorophyll a, herbivorous zooplankton, phosphate, and nitrate for the full and zero measurement cases in each cell. The dots represent the nominal values, the vertical lines to the left of the dots indicate a one standard deviation range for the zero measurement strategy, and the vertical lines to the right give the one standard deviation range for the full measurement case. In some segments the variance grows so rapidly that the zero measurement case gives little information, whereas some predictive capability exists (without measurement) in segment 5. This indicates that it is unacceptable to use uncalibrated models for prediction without supplemental measurements. These measurements of course correspond to what are normally required for model calibration and subsequent verification. The Kalman filter can be used to help define cost-efficient measurement programs.

Figures 10 to 13 show how measurements can be used to improve estimates of the model parameters. The dots represent the best estimate of the parameter before the sampling program, the vertical bars to the left of the dots indicate the one standard deviation range without any measurements, and the vertical bars to the right of the dots indicate the one standard deviation range with a full measurement strategy. Measurements can only improve knowledge of a parameter. Note that in most cases the improvements are better in segment 5 than in segment 1.

The full and zero measurement time history plots for all of the state variables and parameters were used to hypothesize a simple suboptimal measurement strategy. The following guidelines were useful in designing this suboptimal strategy.

(1) Determine the segments in which measurements are the most useful (for example, measurements in segment 5 are preferred to measurements in segment 1).

(2) Determine the earliest time when most of the variance begins noticeable decreases in the parameter plots (for example, in most cases this occurs between $t = 3$ and $t = 6$).

(3) Determine the time region where the maximum variance decrease occurs on most of the seventy-five plots (for example, this occurs most frequently between $t = 6$ and $t = 11$.

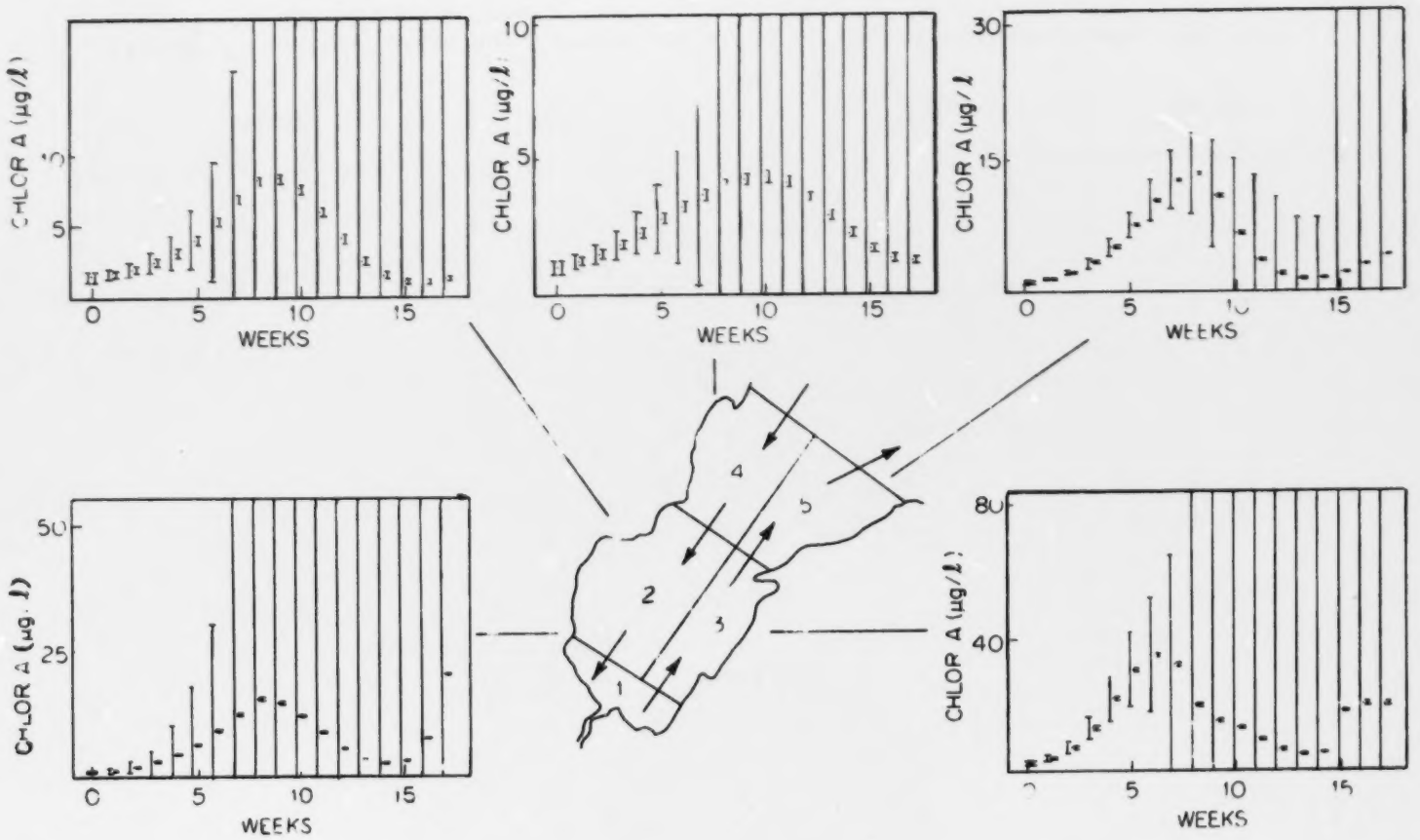

Figure 6. Nominal state and standard deviation for chlorophyll a for full and zero measurement cases.

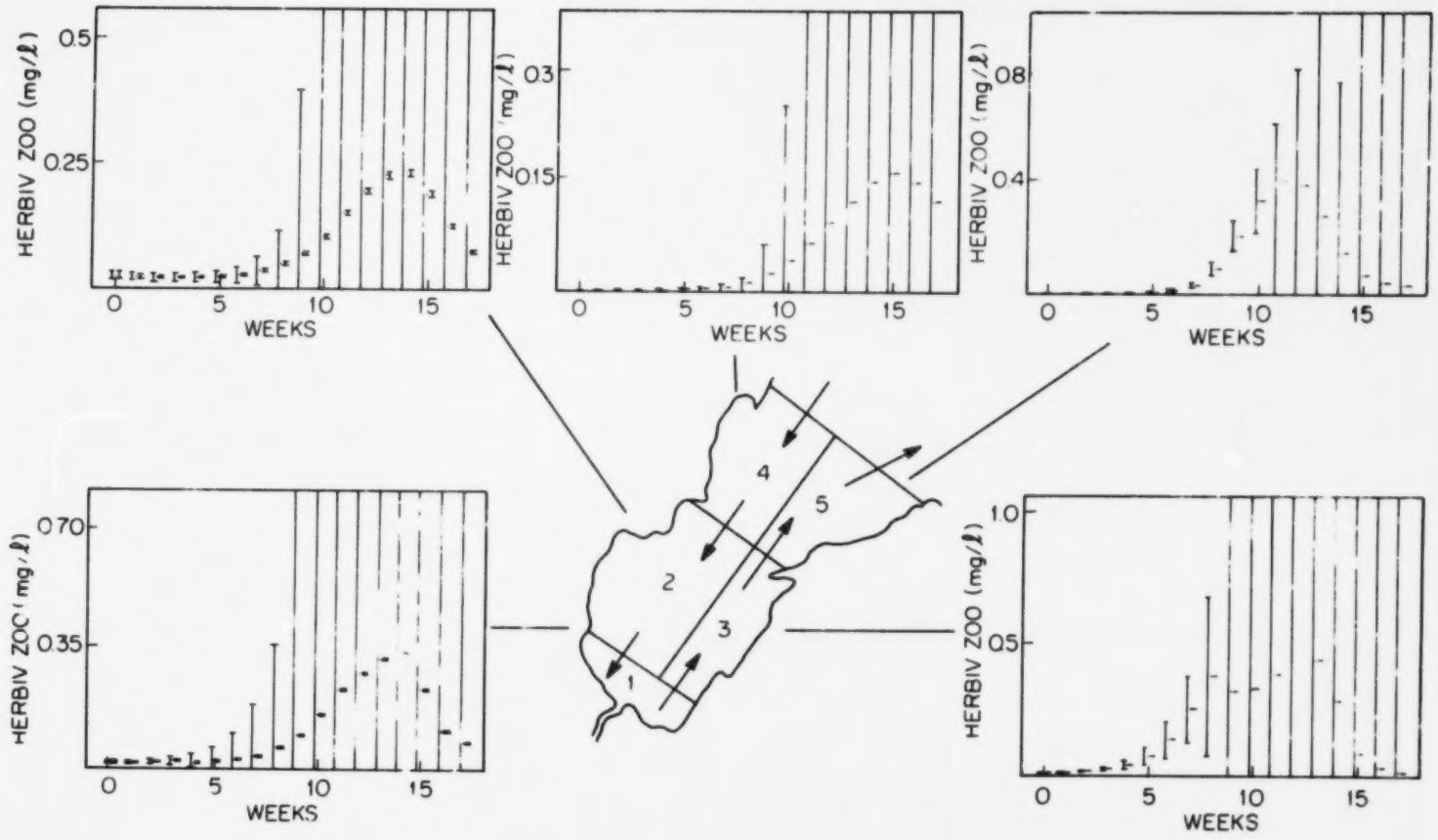

Figure 7. Nominal state and standard deviation for herbivorous zooplankton for full and zero measurement cases.

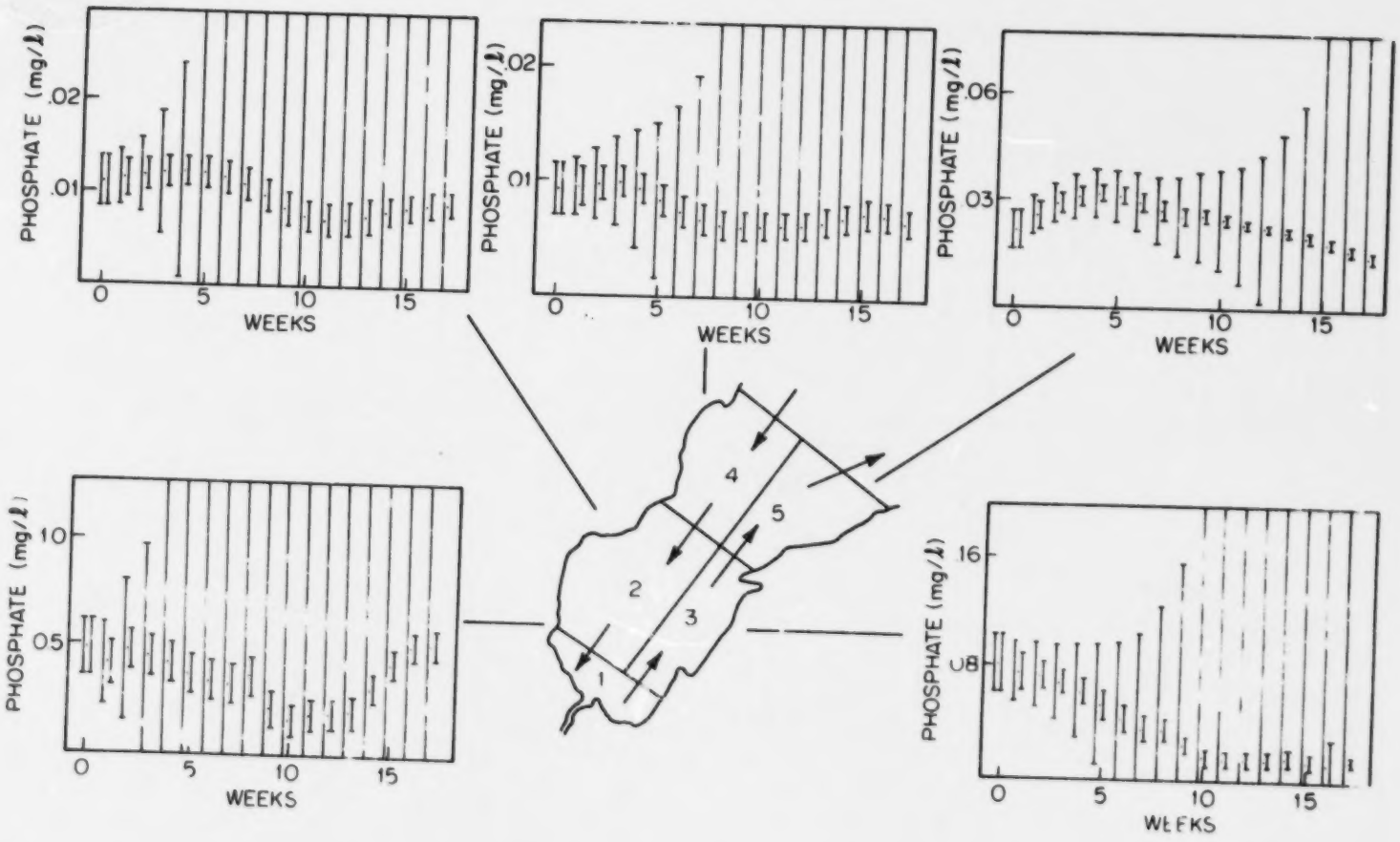

Figure 8. Nominal state and standard deviation for phosphate for full and zero measurement cases.

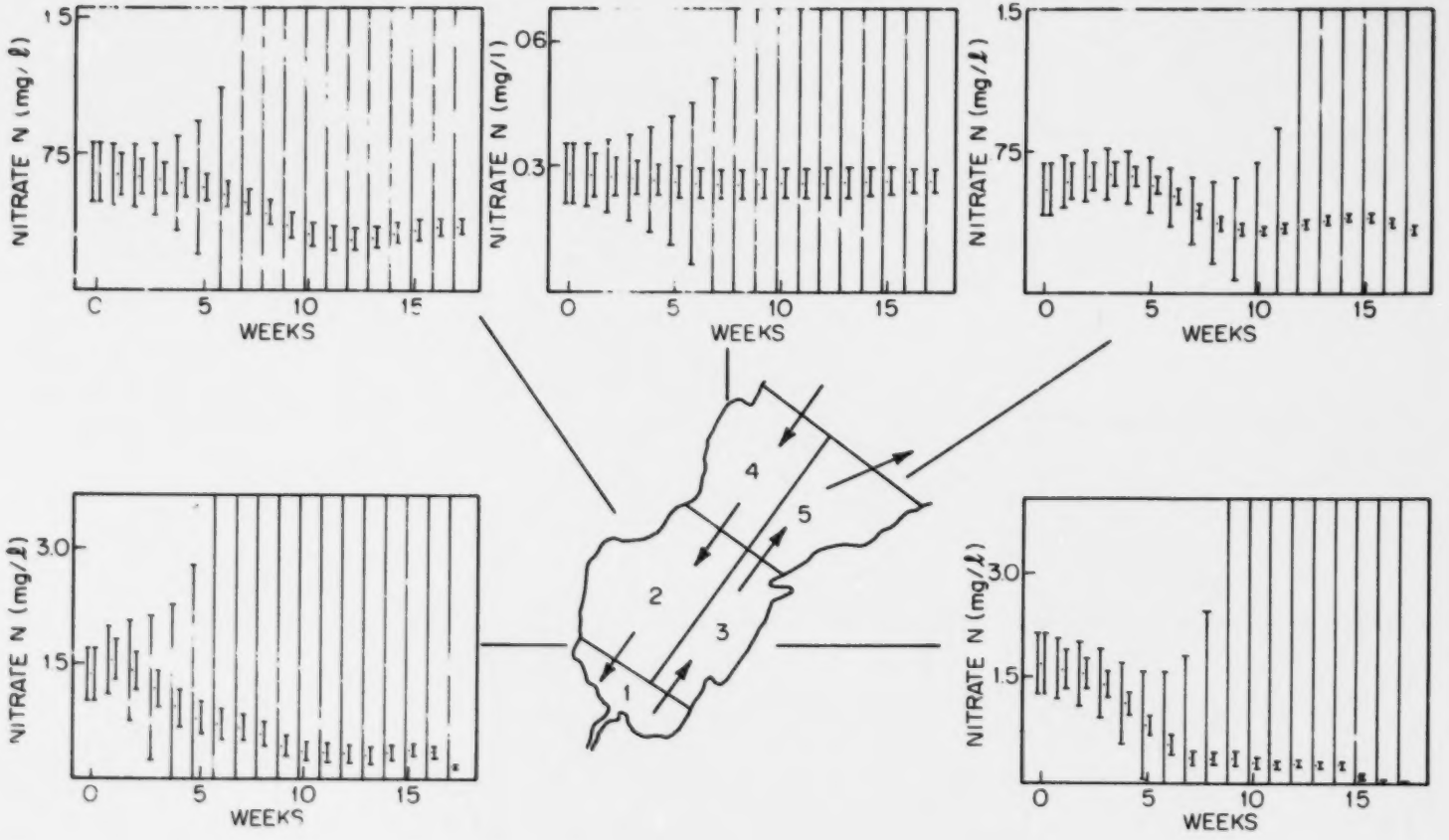

Figure 9. Nominal state and standard deviation for nitrate for full and zero measurement cases.

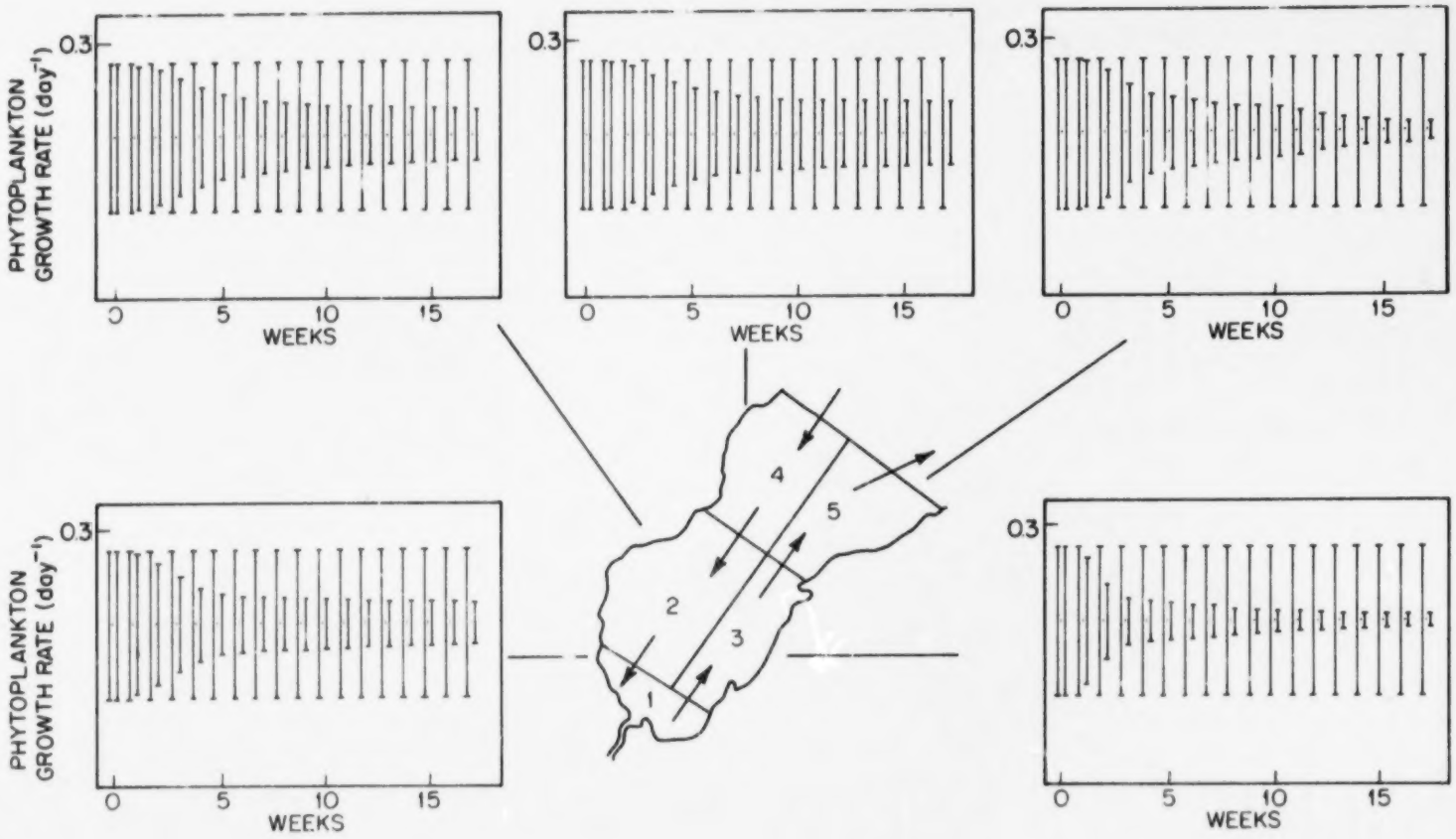

Figure 10. Parameter estimates and standard deviations for the phytoplankton growth rate for full and zero measurement cases.

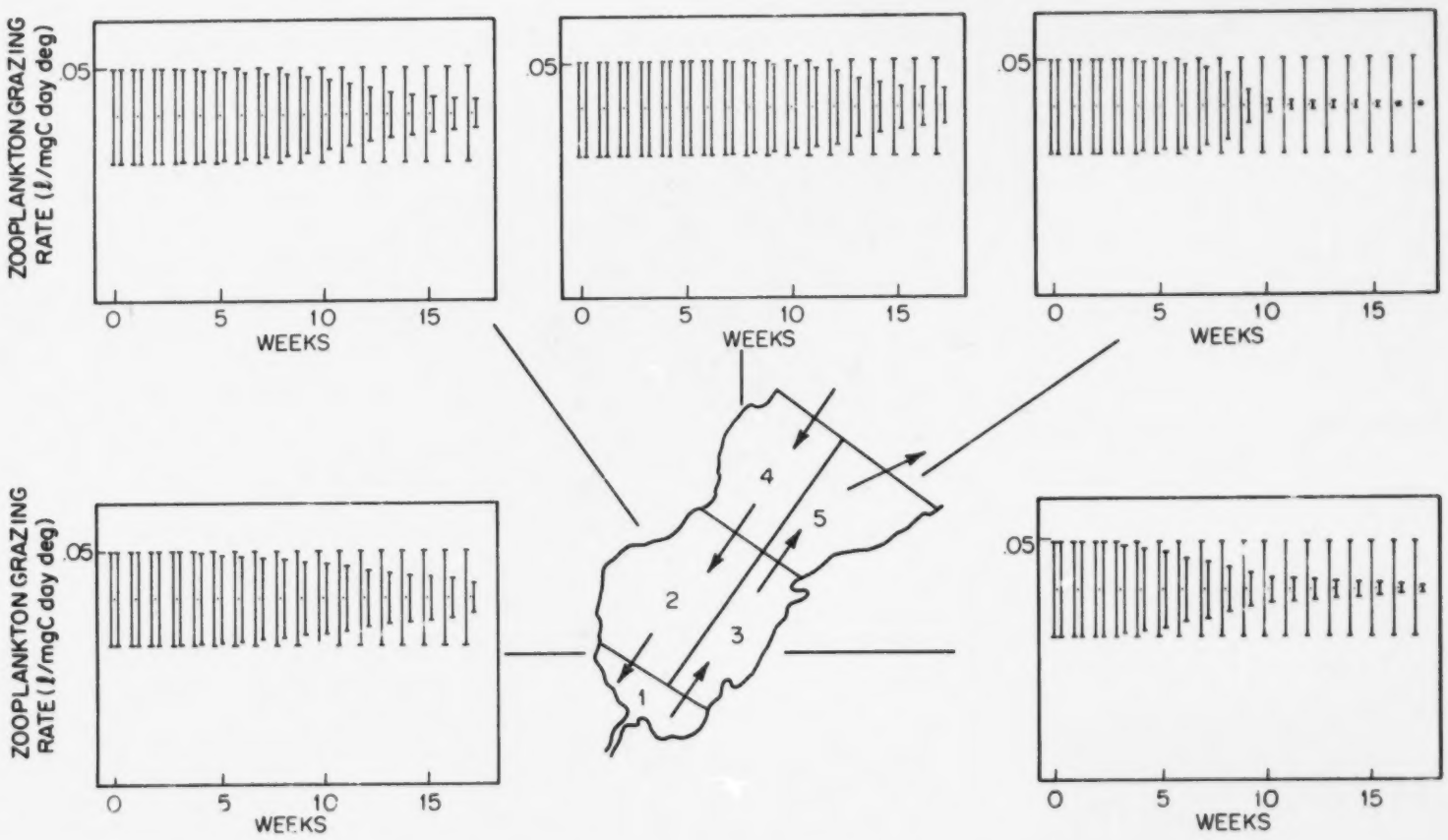

Figure 11. Parameter estimates and standard deviations for the zooplankton grazing rate for full and zero measurement cases.

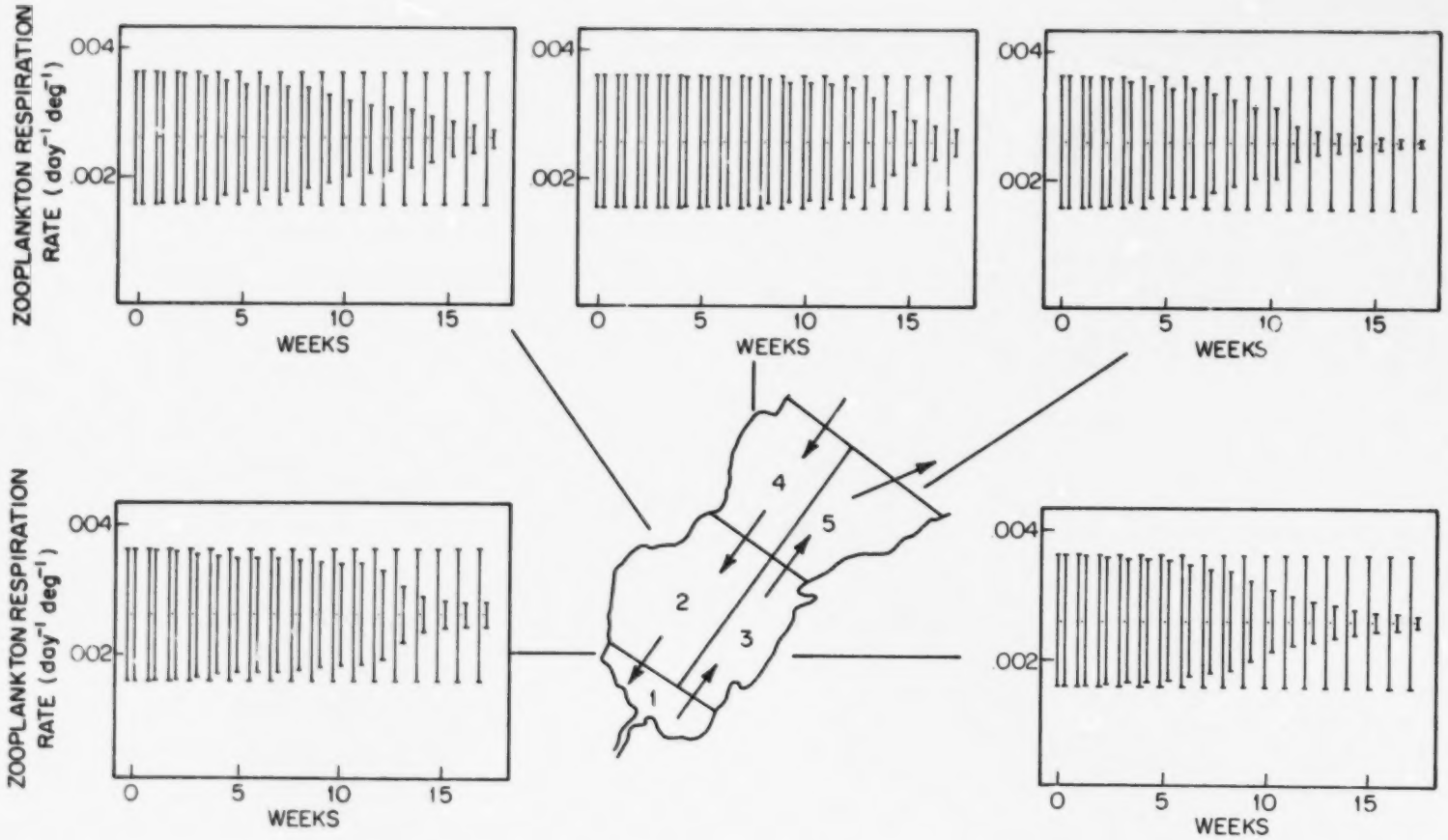

Figure 12. Parameter estimates and standard deviations for the zooplankton respiration rate for full and zero measurement cases.

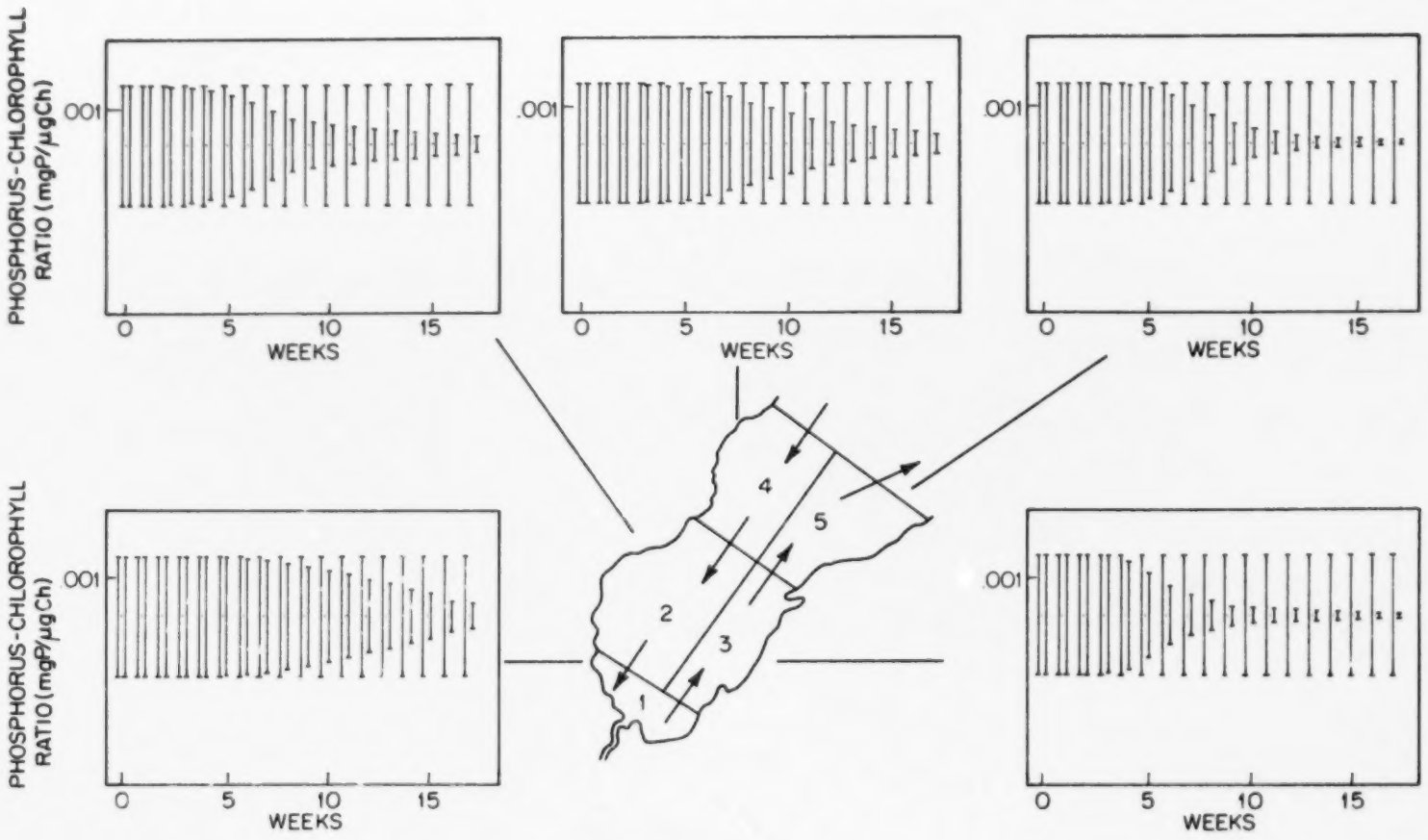

Figure 13. Parameter estimates and standard deviations for the phosphorus-chlorophyll ratio for full and zero measurement cases.

Application of these guidelines suggests a suboptimal sampling program that consists of full measurements only in segments 2 and 5 at t = 3, 8, 9, and 10. The rationale for this strategy is that most of the variances do not start decreasing until t = 3 and that the maximum variance decreases occurred in the region t = 6 and t = 11. Both sides of the bay are sampled because of the segmented structure of the system. Segment 5 is chosen because it gives the most improvements overall, and segment 2 is chosen from the west side because it is connected to two segments. However, estimates from segments 2 and 4 have similar variance levels, so the choice between these segments is somewhat arbitrary. This suboptimal sampling strategy requires approximately 8 percent of the effort of the full measurement strategy.

A summary of some of the major characteristics of the suboptimal strategy (as compared to the full measurement case) is presented in Tables 9 and 10. The current best estimates of the standard deviations of the parameters are shown for all model segments in column (a) of Table 9. The standard deviations attainable with the full measurement strategy are shown in column (b). The standard deviations are reduced by approximately an order of magnitude in segments 3 and 5, whereas approximately a half order of magnitude reduction occurs in segments 1, 2, and 4. Larger reductions in segments 3 and 5 are probably due to the counterclockwise flow pattern in the bay and the structure of the system equations. Thus, for parameter identification, more information is gained from measurements in segments 3 and 5 compared to segments 1, 2, and 4 for the same measurement cost.

The standard deviations for the parameters with the suboptimal measurement strategy are shown in column (c) of Table 9. Substantial reductions in the standard deviations are obtained even though this strategy involves only 8 percent of the effort of the full measurement strategy. Again, the most significant improvements are obtained in segments 3 and 5. It is interesting to note that estimates in segment 3 are more accurate than in segment 2 even though no measurements are performed in segment 3 while measurements are performed in segments 2 at t = 3, 8, 9, and 10.

Important aspects of state variable (as opposed to parameter) estimation are presented in Table 10. Standard deviations of the estimates of chlorophyll a, herbivorous zooplankton, and carnivorous zooplankton at their peak population concentrations are presented for a number of cases. The calculated standard deviation at the peak population in each segment with the full measurement case is given in column (a). Column (b) presents the standard deviations at the peak population with the suboptimal strategy. Suboptimal standard deviations are approximately an order of magnitude larger than the full measurement standard deviations, except for chlorophyll a in segments 2 and 5. Chlorophyll a is estimated more accurately in these segments because the suboptimal strategy involves measurements in segments 2 and 5 during the critical peak growth period for chlorophyll a.

Herbivorous and carnivorous zooplankton are not estimated nearly as accurately as chlorophyll a in segments 2 and 5. The reasons for this are twofold. First, the suboptimal measurement strategy does not contain measurements during the important growth periods for herbivorous and carniv-

TABLE 9. CALCULATED STANDARD DEVIATIONS OF PARAMETER VALUES FOR VARIOUS MEASUREMENT STRATEGIES

Parameter	Cell number	(a) Current estimate	(b) After full measurement	(c) After sub-optimal measurement	(d) After full measurement with improved parameter values	(e) After full measurement with improved initial conditions
Phytoplankton saturated growth rate	1	.0910	.0236	.0433	.00581	.0160
Phytoplankton respiration rate	1	.0225	.0147	.0193	.00200	.0109
Zooplankton grazing rate	1	.0100	.0027	.00699	.000756	.00215
Zooplankton respiration rate	1	.0011	.00019	.00064	.000722	.000114
Carbon to chlorophyll ratio	1	.0200	.00377	.00953	.000998	.00252
Nitrogen to chlorophyll ratio	1	.00175	.00085	.00138	.000145	.000714
Phosphorus to chlorophyll ratio	1	.00031	.000056	.0000230	.0000230	.0000370
Phytoplankton saturated growth rate	2	.0910	.0295	.0428	.00694	.0217
Phytoplankton respiration rate	2	.0225	.0118	.0165	.00199	.00887
Zooplankton grazing rate	2	.0100	.00277	.00649	.000755	.00214
Zooplankton respiration rate	2	.0011	.000112	.000472	.0000520	.0000779
Carbon to chlorophyll ratio	2	.0200	.00402	.0103	.00118	.00319
Nitrogen to chlorophyll ratio	2	.00175	.000844	.00125	.000149	.000707
Phosphorus to chlorophyll ratio	2	.00031	.0000376	.000160	.0000188	.0000290
Phytoplankton saturated growth rate	3	.0910	.00647	.0187	.00269	.00318
Phytoplankton respiration rate	3	.0225	.00544	.0129	.00176	.00235
Zooplankton grazing rate	3	.0100	.00067	.00302	.000383	.000499
Zooplankton respiration rate	3	.0011	.000088	.000419	.0000555	.0000577
Carbon to chlorophyll ratio	3	.0200	.00099	.00512	.000623	.000777
Nitrogen to chlorophyll ratio	3	.00175	.000267	.000942	.000110	.000160
Phosphorus to chlorophyll ratio	3	.00031	.000013	.0000407	.0000081	.0000073

(Continued)

TABLE 9. (Continued)

Parameter	Cell number	(a) Current estimate	(b) After full measurement	(c) After sub-optimal measurement	(d) After full measurement with improved parameter values	(e) After full measurement with improved initial conditions
Phytoplankton saturated growth rate	4	.0910	.0379	.0694	.00836	.0250
Phytoplankton respiration rate	4	.0225	.0120	.0173	.00194	.0101
Zooplankton grazing rate	4	.0100	.00322	.00700	.000790	.00244
Zooplankton respiration rate	4	.0011	.000180	.00062	.0000670	.000144
Carbon to chlorophyll ratio	4	.0200	.00584	.0136	.00145	.00459
Nitrogen to chlorophyll ratio	4	.00175	.00101	.00143	.000152	.000919
Phosphorus to chlorophyll ratio	4	.00031	.000049	.00014	.0000218	.000036
Phytoplankton saturated growth rate	5	.0910	.00994	.0217	.00397	.00685
Phytoplankton respiration rate	5	.0225	.00347	.00839	.00140	.00216
Zooplankton grazing rate	5	.0100	.00036	.000705	.000231	.000288
Zooplankton respiration rate	5	.0011	.000049	.000213	.0000286	.0000375
Carbon to chlorophyll ratio	5	.0200	.000715	.00186	.000517	.000578
Nitrogen to chlorophyll ratio	5	.00175	.000268	.000592	.000111	.000214
Phosphorus to chlorophyll ratio	5	.00031	.0000104	.0000295	.0000064	.0000059

TABLE 10. CALCULATED STANDARD DEVIATIONS OF PEAK POPULATIONS FOR VARIOUS MEASUREMENT STRATEGIES

State Variables	Model cell number	Time of peak (weeks)	(a) After full measurement	(b) After sub-optimal measurement	(c) After full measurement with improved parameter values	(d) After full measurement with improved initial conditions
Chlorophyll a	1	8	0.237	2.240	0.233	0.235
Herbivorous zooplankton	1	14	0.00381	0.0359	0.00362	0.00378
Carnivorous zooplankton	1	17	0.00180	0.0176	0.00178	0.00180
Chlorophyll a	2	9	0.310	0.341	0.281	0.300
Herbivorous zooplankton	2	14	0.00585	0.0475	0.00517	0.00551
Carnivorous zooplankton	2	17	0.00190	0.0174	0.00181	0.00188
Chlorophyll a	3	6	0.494	3.335	0.423	0.471
Herbivorous zooplankton	3	13	0.00311	0.0297	0.00304	0.00310
Carnivorous zooplankton	3	16	0.00165	0.0160	0.00163	0.00164
Chlorophyll a	4	10	0.204	1.421	0.185	0.192
Herbivorous zooplankton	4	15	0.000206	0.00203	0.000204	0.000205
Carnivorous zooplankton	4	17	0.0000648	0.000643	0.0000647	0.0000647
Chlorophyll a	5	8	0.196	0.227	0.169	0.193
Herbivorous zooplankton	5	11	0.000742	0.00559	0.000721	0.00738
Carnivorous zooplankton	5	15	0.000215	0.00208	0.000212	0.000214

orous zooplankton. Second, the variances for these two state variables change most rapidly for $t > 10$, but the suboptimal measurement strategy does not include measurements after $t = 10$. If peak population prediction of zooplankton is desired, the measurements at $t = 8$ and 10 should probably be eliminated and replaced by measurements $t = 11$ and $t = 17$. In such a case, the suboptimal strategy would consist of full measurements at $t = 3$, 9, 11, and 17.

It is also of interest to determine how the uncertainty of model states changes when knowledge of the model initial states and parameters improves when a full measurement strategy is employed. The first case involves full measurements with an order of magnitude reduction in the initial standard deviations of the parameters. The second case considers full measurements with an order of magnitude reduction in the initial standard deviations of the state variables. Physically, the first case corresponds to a systematic improvement of the parameter values. This might occur during the season year of a sampling program if the first year of monitoring resulted in an order of magnitude reduction of the parameter standard deviations, or it could occur as a consequence of laboratory or field experiments. Case 2 could correspond physically to a situation where an extensive initial sampling effort allows the standard deviations of the state variables to be reduced by an order of magnitude.

The results of these cases are summarized in columns (d) and (e) of Table 9 and columns (c) and (d) of Table 10. A comparison of the results in columns (d) and (e) with column (b) in Table 9 indicates that standard deviations are reduced by approximately a factor of two to four and that improvements of parameters gives somewhat better results than improvements of initial conditions for parameter estimation accuracy. It is interesting to note that the peak concentration standard deviations are approximately the same for all three full-measurement cases (see Table 10). Thus, an order of magnitude reduction in the initial parameter or state variable standard deviations does not increase the capability of making more accurate peak value predictions. This is probably because of large increases in the standard deviations of chlorophyll a, carnivorous zooplankton, and herbivorous phytoplankton during critical growth periods, and only measurements in these regions can insure reasonably accurate values. This is in sharp contrast to the results presented earlier with no measurements where improvements in the state initial conditions and parameter values significantly reduce the calculated standard deviation at the peak populations (see Table 8).

SUMMARY

This section contains a preliminary investigation of the potential applicability of Kalman filtering techniques for concentration and parameter identification associated with a phytoplankton and nutrient cycling model for Saginaw Bay. It has been determined that the accuracy of uncalibrated model predictions is limited. Therefore, field monitoring and laboratory research programs are necessary to improve model predictive capabilities. Cost-effective monitoring programs must be designed using trail-and-error optimization rather than automatic optimization because of the relatively

large number of differential equations required to describe the annual nutrient and plankton cycles.

A suboptimal, but effective, sampling program has been developed to improve the accuracy of the model calculations. An example monitoring program for Saginaw Bay involves approximately 8 percent of the maximum number of samples. it has been determined that this sampling program applied in the context of the Kalman filter and the system model can significantly reduce the uncertainty associated with predicted values of the state variables such as chlorophyll a. Several tables are presented showing these results. Although the limited analyses in this study are preliminary and incomplete, it is concluded that Kalman filtering techniques can be applied to determine the accuracy of limnological model predictions as a function of the uncertainties associated with the model parameters or coefficients and initial conditions. If the accuracy of such models is unacceptable, even with good knowledge of parameters and initial conditions, it may be necessary to supplement model predictions with field measurements of the concentrations. In these cases, Kalman filtering and optimization techniques can be used to determine efficient and cost-effective monitoring programs.

REFERENCES

Beck, B., and P.C. Young. 1976. Systematic Identification of DO-BOD. Journal of the Environmental Engineering Division, Vol. 102, No. EE5, pp. 909-927.

Canale, R.P., L.M. DePalma, and A.H. Vogel. 1976. A Plankton-Based Food Web Model for Lake Michigan. In: Modeling Biochemical Processes in Aquatic Ecosystems, R.P. Canale, ed., Ann Arbor Science, Ann Arbor, Michigan.

Chapra, S.C. 1975. Comment on an Empirical Method of Estimating the Retention of Phosphorus in Lakes by W.B. Kirchner and P.J. Dillon. Water Resources Res., 11: 1033-1034.

Chapra, S.C. 1977. Total Phosphorus Model for the Great Lakes. ASCE J. Environmental Engr. Division, Vol. 103, No. EE2, pp. 147-161.

Davenport, W.B., Jr. 1970. Probability and Random Processes. McGraw-Hill, New York. 542 pp.

DePalma, L.M. 1977. A Class of Measurement Strategy Optimization Problems--with an Application to Lake Michigan Surveillance. Ph.D. dissertation, University of Michigan, Ann Arbor, Michigan. 122 pp.

Dillon, P.J. and W.B. Kirchner. 1975. Reply to Chapra (1975). Water Resources Res., 11: 1035-1036.

Gelb, A. 1974. Applied Optimal Estimation. MIT Press, Cambridge, Massachusetts. 374 pp.

Great Lakes Water Quality Board. 1976. International Surveillance Program for the Great Lakes. In: 1975 Annual Report, Great Lakes Water Quality, Appendix B, Windsor, Ontario, Canada. 255 pp.

Harrison, M.J., R.E. Pacha, and R.Y. Morita. 1972. Solubilization of Inorganic Phosphates by Bacteria Isolated from Upper Klamath Lake Sediment. Limnology and Oceanography., 17: 50-57.

Hutchinson, G.E. 1957. A Treatise on Limnology, Vol. 1. John Wiley and Son, New York. 1015 pp.

Jazwinski, A.H. 1970. Stochastic Processes and Filtering Theory. Academic Press, New York. 376 pp.

Junge, C.E. and R.T. Werby. 1958. The Concentration of Chloride, Sodium, Potassium, Calcium and Sulfate in Rain Water over the United States. J. Meterology., 15: 417-425.

Kalman, R.E. 1960. A New Approach to Linear Filtering and Prediction Problems. Trans. ASME, J. Basic Engr., 82D: 34-35.

Kalman, R.E. and R. Bucy. 1961. New Results in Linear Filtering and Prediction Theory. Trans. ASME, J. Basic Engr., 83D: 95-108.

Kirchner, W.B. and P.J. Dillon. 1975. An Empirical Method of Estimating the Retention of Phosphorus in Lakes. Water Resources Res., 11: 182-183.

Krogh, F.T. 1969. VODQ/SVDQ/DVDQ - Variable Order Intergrators for the Numerical Solution of Ordinary Differential Equations. Jet Propulsion Laboratory TU Document No. CP-2308, NPO-11643. 22 pp.

Larsen, D.P. and H.J. Mercier. 1976. Phosphorus Retention Capacity of Lakes. J. Fisheries Res. Board of Canada., 33: 1742-1750.

Lorenzen, M.W., D.J. Smith, and L.V. Kimmel. 1976. A Long-Term Phosphorus Model for Lakes: Application to Lake Washington. In: Modeling Biochemical Processes in Aquatic Ecosystems, R.P. Canale, ed., Ann Arbor Science, Ann Arbor, Michigan.

Michalski, M.F.P., M.G. Johnson, and D.M. Veal. 1973. Muskoka Lakes Water Quality Evaluation, Report No. 3: Eutrophication of the Muskoka Lakes. Ontario Ministry of the Environment, Toronto, Ontario, Canada. 57 pp.

Moore, S.F. 1971. The Application of Linear Filter Theory to the Design and Improvement of Measurement Systems for Aquatic Environment. Ph.D. Dissertation, University of California at Davis, California. 218 pp.

Murphy, T.J. and P.V. Doskey. 1975. Inputs of Phosphorus from Precipitation to Lake Michigan. EPA-600/3-75-005, U.S. Environmental Protection Agency, Duluth, Minnesota. 27 pp.

O'Connor, D.J. and J.A. Mueller. 1970. A Water Quality Model of Chloride in Great Lakes. ASCE J. Sanitary Engr. Div., 4: 955-975.

Quinn, F.H. 1975. Lake Michigan Beginning-of-Month Water Levels and Monthly Rates of Change of Storage. National Oceanic and Atmospheric Administration Report No. TRERL326-GLERL2, Boulder, Colorado. 32 pp.

Quinn, F.H. 1977. Annual and Seasonal Flow Variations through the Straits of Mackinac. Water Resources Res., Vol. 13, 137-144.

Richardson, W.L. and V.J. Bierman, Jr. 1976. A Mathematical Model of Pollutant Cause and Effect in Saginaw Bay, Lake Huron. In: Water Quality Criteria Research of the USEPA, EPA-600/3-76-079, Corvallis, Oregon. pp. 138-158.

Sage, A.P. and J.L. Melsa. 1971. Estimation Theory with Applications to Communications and Control. McGraw-Hill, New York. 529 pp.

Saylor, J.H. and P.W. Sloss. 1976. Water Volume Transport and Oscillatory Current Flow through the Straits of Mackinac. J. Physical Oceanography, Vol. 6, 229-237.

Sonzogni, W.C. 1974. Effect of Nutrient Input Reduction on the Eutrophication of the Madison Lakes. Ph.D. Dissertation, University of Wisconsin, Madison, Wisconsin. 352 pp.

Stewart, K.M. and S.J. Markella. 1974. Seasonal Variations in Concentrations of Nitrate and Total Phosphorus and Calculated Nutrient Loading for Six Lakes in Western New York. Hydrobiologia., 44: 61-89.

Thomann, R.E., D.M. DiToro, R.P. Winfield, and D.J. O'Connor. 1975. Mathematical Modeling of Phytoplankton in Lake Ontario - 1. Model Development and Verification. EPA-660/3-75-005, U.S. Environmental Protection Agency, Corvallis, Oregon. 177 pp.

U.S. Army Corps of Engineers. 1975. Lake Erie Wastewater Management Study: Preliminary Feasibility Report, Buffalo, New York. 167 pp.

APPENDIX A

DISCRETE KALMAN FILTER AND OPTIMIZATION OF MEASUREMENT STRATEGIES

INTRODUCTION

The Kalman filter equations for a scalar differential equation process model with discrete, full state measurements were presented in Section 4 to develop insight into the basic procedure. In this appendix, the Kalman filter equations for a discrete process model (for example, the discretization of a system of differential equations by numerical integration formulas) and discrete measurements will be presented along with the method employed to minimize the cost subject to constraints on the state estimate variance.

DISCRETE KALMAN FILTER

In this section, the process model is assumed to be of the form

$$x(k+1) = \phi_k\, x(k) + w(k),\ (k = 0,1,\ldots,k) \qquad (A.1)$$

where x(k) is an n-vector describing the state at index k (for example, time t_k), ϕ_k is an nxn matrix describing the known relation between the state at x(k) and x(k+1), and w(k) is the model equation error at k (for example, model inadequacy, lack of knowledge of parameters in ϕ_k, etc). (Since the index k is usually associated with time, k will usually be referred to as time instead of index.) Equation (A.1) is a linear difference equation; however, most water quantity models are nonlinear. The Kalman filter and optimization equations will be presented for the linear system of Equation (A.1). It will be shown how to transform nonlinear water quality process models into the form of Equation (A.1) later in this section.

Equation (A.1) may result naturally (for example, in Section 5 a discrete model is employed to describe year-to-year changes of phosphorus, chloride, and sinking rate) or from a discretization of a differential equation model (for example, in Section 6 the LAKE-1 differential equation model is discretized to form a system of difference equations).

As with the development of Section 4, to apply the Kalman filtering approach to Equation (A.1), statistics associated with the initial state, x(o), and the model error, w(k), must be supplied. Again it is assumed that the model error is zero-mean, sequentially uncorrelated (white) noise, that is,

$$E\left[w(k)\right] = 0 \quad , \quad E\left[w(k)w(j)^T\right] = Q(k)\delta_{kj} \tag{A.2}$$

where $\delta_{kj} = \begin{cases} 1, & k=j \\ 0, & k\neq j \end{cases}$, and the initial state statistics are

$$E\left[x(o)\right] = \hat{x}_o \quad , \quad P_o = E\left[(x(o)-\hat{x}_o)(x(o)-\hat{x}_o)^T\right]. \tag{A.3}$$

In Section 4 it was assumed that the full state was measured at each measurement time. In this section, the general situation in which measurements of linear combinations of the states are made at certain times is considered. A linear combination of states at time k is a weighted sum of the individual states. If a row vector C_m is introduced to write concisely this weighted sum, then a measurement of type m at time n may be denoted

$$y_{mk} = C_m\, x(k) + v_{mk}, \tag{A.4}$$

where y_{mk} is the scalar measurement of the linear combination $C_m\, x(k)$ and v_{mk} is the associated measurement error with

$$E\left[v_{mk}\right] = 0 \quad , \quad E\left[v_{mk}^2\right] = R_{mk} \, . \tag{A.5}$$

If at any time k all states are measured, then the C_m set is the identity matrix. If M types of measurements are made at each time k = 1, ..., N, then M times N measurements are made in total. As an example of this notation, consider an eutrophication model with states x_1, ..., x_8 corresponding to the eight water quality variables: phytoplankton, zooplankton, dissolved phosphorus, particulate phosphorus, nitrate, ammonia, organic nitrogen, and silicon, respectively. The measurement type corresponding to a measurement of only zooplankton biomass would be

$$C_1 = [0\ 1\ 0\ 0\ 0\ 0\ 0\ 0], \tag{A.6}$$

and the type corresponding to a Kjeldahl nitrogen measurement (ammonia plus organic nitrogen would be

$$C_2 = [0\ 0\ 0\ 0\ 0\ 1\ 1\ 0]. \tag{A.7}$$

The error variance for a measurement of type m at time k, R_{mk}, depends on the number of vertical hauls made at the station. The variance of a total phosphorus measurement would depend on the number of subsample digested and analyzed.

The Kalman filter combines the information provided by the model in Equation (A.1 - A.3) and the measurements in Equations (A.4 and A.5) to compute the conditional mean estimate of the system state, denoted by $\hat{x}(k)$, which is the estimate based on all measurements taken prior to and at time

k.[1] The filter is recursive in that it permits $\hat{x}(k)$ to be computed from $\hat{x}(k-1)$ and the measurement vector at time k. Recursive estimation is a common procedure, for example, least squares curve fitting is commonly formulated recursively so that each data point is processed as it is received rather than the data being batch processed when all are available.

As in Section 4, the Kalman filter equations are applied recursively in two stages. Given $\hat{x}(k-1)$, $P(k-1)$, the first involves the propagation of $\hat{x}$ and P to the next measurement time, k. The state prediction is simply the difference equation without the model error, that is,

$$\hat{x}(k^-) = \phi_{k-1}\, \hat{x}(k-1), \tag{A.8}$$

and the covariance propagation is

$$P(k^-) = \phi_{k-1} P(k-1) \phi_{k-1}^T + Q(k-1), \tag{A.9}$$

which has an interpretation analogous to Equation (4.8) in Section 4, that is, the covariance is influenced by the dynamics through the first term and the model inadequacy through the second term of Equation (A.9).

The second stage involves processing the measurement at time k, and the equations are essentially the same as Equations (4.6 - 4.8) in Section 4 since discrete measurements were assumed there. In particular

$$P(k) = \left[I + \sum_{m=1}^{M} \frac{C_m^T C_m}{R_{mk}} \right]^{-1} P(k^-) \quad \text{and} \tag{A.10}$$

$$\hat{x}(k) = \hat{x}(k^-) + P(k) \sum_{m=1}^{M} \frac{C_m^T}{R_{mk}} \left[y_{mk} - C_m\, \hat{x}(k^-) \right] . \tag{A.11}$$

The difference between these equations and Equations (4.6 - 4.8) result from the following: the special way that the measurements are treated at each k in Equation (A.4) (that is, as a set of scalar measurements); the fact that a full state measurement is not assumed; and, because this form is more convenient for the measurement strategy optimization problem. Also, because the measurements are treated as a set of scalar measurements at a given k (which is advantageous for optimization of measurement strategy purposes), the Kalman gain provides little insight for this case and is not introduced. As with the case of Section 4, note that if R_{mk} is relatively large (indicating a relatively bad measurement), then the coefficient of $P(k^-)$ in Equation (A.10) is approximately I, which implies $P(k) \approx P(k^-)$, that is, the

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[1] In this section, $\hat{x}(k)$ is analogous to $\hat{x}(t_k^+)$ of Section 4. The + sign is not employed because it becomes awkward for indices of the form k-1, k+1, etc.

measurement has little influence. Conversely, if the R_{mk} are relatively small, the inverse of

$$I + \sum_{m=1}^{T} C_m^T C_m / R_{mk}$$

will also be relatively small, which results in a reduction of $P(k^-)$ in forming $P(k)$.

MEASUREMENT STRATEGY OPTIMIZATION

It is evident from Equation (A.11) that the estimate for $x(k)$ for all $k = 1, \ldots, K$ cannot be computed until the measurements have been taken, that is, until y_{mk} are available for each $m = 1, \ldots, M$ and $k = 1, \ldots, K$. However, the accuracy of the estimates, which is manifested in the covariance matrix $P(k)$ for $k = 1, \ldots, K$, can be precomputed from Equations (A.9) and (A.10) once the necessary matrices, vectors, and scalars have been specified. This point is vital to the technique for definition of optimal measurement strategies. The estimation error covariance matrices $P(k)$ can be computed for every $k = 1, \ldots, K$ once the measurement strategy has been specified for $k = 1, \ldots, K$. Computation need not wait until the actual measurements have been taken. The Kalman filter exhibits this property because the statistics of model uncertainty and measurement uncertainty are not computed during the processing but rather are assumed known prior to time zero. The manner in which the statistics might be quantified are demonstrated in the applications in Sections 5 and 6.

The vector estimates, $\hat{x}(k)$, for $k = 1, \ldots, K$ are comprised of n individual state estimates $\hat{x}_i(k)$ for $i = 1, \ldots, n$. The accuracy of $\hat{x}_i(k)$ is reflected in the estimation error variance of $\hat{x}_i(k)$, that is the ith diagonal entry of the estimation error covariance matrix $P(k)$. It is of considerable interest to investigate the effect of the measurement strategy on the variances $P_{ii}(k)$. In particular, it may be of interest to calculate the minimum-cost measurement strategy that satisfies constraints

$$P_{ii}(k) \leq Pmax_{ik} \text{ for } i = 1, \ldots, n \text{ and } k = 1, \ldots, K. \qquad (A.12)$$

In Equation (A.12), $P_{ii}(k)$ is a scalar, and the $Pmax_{ik}$ are bounds that are imposed to guarantee that the resulting estimates of $\hat{x}_i(k)$ are of sufficient accuracy to serve some purpose. In Section 5, for example, values of $Pmax_{ik}$ are chosen to guarantee that the state estimates will be accurate enough for long-term pollutant trend detection.

The optimization problem of this section will be formulated to be compatible with DePalma (1977). In order to accomplish this, assume that a measurement y_{mk} is actually the arithmetic average of a number of multiple measurements. In particular, suppose L_k multiple measurements are made of the form

$$y^i = C_m x(k) = r^i \quad \text{for} \quad i = 1, \ldots, L_k \qquad (A.13)$$

where r^i is a measurement error (associated with y^i) and zero mean and variance R_m. The resultant measurement is the arithmetic average of these L_k measurements, or

$$y_{mk} = \frac{1}{L_k} \sum_{i=1}^{L_k} y^i = C_m x(k) + \frac{1}{L_k} \sum_{i=1}^{L_k} r^i \quad . \tag{A.14}$$

If the correspondence

$$r_{mk} = \frac{1}{L_k} \sum_{i=1}^{L_k} r^i \tag{A.15}$$

is made, then Equations (A.4) and (A.14) are equivalent. Furthermore, if r^i are independent random variables, then the variance of the resultant measurement error is inversely proportional to L_k,

$$R_{mk} = R_m/L_k. \tag{A.16}$$

For many types of measurements, the number of multiple measurements is limited by such practical considerations as the number of stations that can be sampled in one day or the number of analyses a laboratory can schedule. For such situations in which each measurement must be computed from no more than Lmax multiple measurements,

$$0 \leq L \leq \text{Lmax for each } k = 1, \ldots, K. \tag{A.17}$$

Furthermore, the cost of multiple measurements is usually proportional to the number of multiple measurements. Therefore, the total cost of a measurement strategy would be

$$\sum_{k=1}^{K} \alpha L_k \tag{A.18}$$

where α is the cost of taking one measurement of each type $m = 1, \ldots, M$. The unit cost α and the maximum number of multiple measurements Lmax are assumed not to be functions of time k.

In the optimization problem, L_k is interpreted as a variable that can be chosen from the interval defined by Equation (A.17). Besides having control over the measurement strategy, it may be desirable to control the model error covariance matrices defined by Equation (A.9). The motivation for the formulation that follows is the trend detection problem examined in Section 5. In that problem, one component of model error is caused by tributary load uncertainty. The variance of this error, however, depends upon the number of days for which the tributaries are sampled. In this optimization problem, both a measurement strategy (in the sense defined in the preceding

paragraph) and a tributary sampling program will be sought that minimize cost and satisfy Equation (A.12).

First, define an nxn matrix at each time k

$$\Omega(k) = Q(k) \tag{A.19}$$

and consider a situation in which $\Omega(k)$ may be decomposed into the sum of an uncontrollable matrix $\Omega^U(k)$ and a controllable matrix $\Omega^C(k)$. Furthermore, assume that only the diagonal elements of $\Omega^C(k)$ can be controlled and that other elements are zero. DePalma (1977) has demonstrated that the error variances of tributary load estimates can be interpreted as the diagonal entries $\Omega^C_{ii}(k)$ of a controllable matrix $\Omega^C(k)$. Control over these elements is feasible if it is possible to control the number of days, D_k, for which tributary water samples are collected. A cost of D_k will be assigned to the tributary sampling program. The total cost, over K years, is then

$$\sum_{k=1}^{K} \beta D_k \tag{A.20}$$

The optimization problem considered by DePalma (1977) requests the measurement strategy (L_k for k = 1, ..., K) and the number of days (D_k for k = 0, ..., K-1) which minimizes the total cost (sum of Equations (A.18) and (A.20)) subject to constraints on estimation error variances defined by Equation (A.12). An algorithm is described by DePalma (1977) to solve this problem, and it is applied to the trend detection problem of Section 5. The theory behind the algorithm utilizes the theory of mathematical programming and will not be presented here.

APPLICATION TO NONLINEAR MODELS

In the previous sections of this appendix, only linear models were employed as a source of information to estimate the state of a physical system. Most physical systems, including the water resource systems examined in this report, cannot be described adequately by a linear model with additive modeling uncertainties. In general, the system state at time k+1, X(k+1), is a nonlinear function of the state at time k, X(k), and the uncertainty in this transition cannot be interpreted as additive. A very general nonlinear stochastic difference equations of the form

$$X(k+1) = f_k[X(k), W(k)] \tag{A.21}$$

will be considered where f is a vector of n nonlinear functions, each dependent on some or all of the states X(k) and the uncertainties W(k). The initial state and the random uncertainties have means and covariance matrices $\bar{X}(0)$, $\bar{W}(k)$, P(0), and Q(k), (k = 1, ..., K), respectively.

The Kalman filter is a scheme for computing the conditional mean estimate of X(k), based on a linear model and measurements. Exact schemes for

computing the conditional mean of X(k) for a nonlinear model have not yet been developed. Approximate schemes have been derived and are presented in Sage and Melsa (1971). Most of these methods solve two couple difference equations, one for an approximate conditional mean $\hat{X}(k)$ and the other for an approximate estimation error covariance matrix P(k) associated with $\hat{X}(k)$. Because the equations are coupled and $\hat{X}(k)$ depends upond the actual measurement values, the covariance matrix P(k) also depends upon the actual measurement values, the covariance matrix P(k) also depends on the measurements. Therefore, P(k) for k = 1, ..., K cannot be precomputed, even if the measurement strategy has been specified prior to time zero. Because of this limitation, these methods for approximating the conditional mean will not be considered further in this report.

However, a method has been proposed (the linearized Kalman filter) for which the approximate estimation error covariance matrix can be precomputed and is not dependent on the actual measurements. Rather than X(k) being estimated directly, the deviation of X(k) from a nominal state Xnom(k) is estimated. The nominal state is that which one would expect if random model uncertainties W(k) were known (and were equal to their means) and the initial state was equal to its mean. The nominal is computed by

$$\text{Xnom}(k+1) = f_k[\text{Xnom}(k), \bar{W}(k)], \tag{A.22}$$

which employs the full nonlinear model with $\text{Xnom}(0) = \bar{X}(0)$. The deviation of the state from the nominal is defined by

$$x(k) = X(k) - \text{Xnom}(k). \tag{A.23}$$

A linear approximation to the dynamics of x(k) can be derived by expanding f_k in a Taylor series and ignoring terms of order two or higher. In order to simplify notation, the vectors of partial derivatives are denoted by

$$f_k x_i \equiv \partial f_k / \partial x_i(k) \Big|_{\substack{\text{Xnom}(k) \\ \bar{W}(k)}}$$

$$f_k w_i \equiv \partial f_k / \partial w_i(k) \Big|_{\substack{\text{Xnom}(k) \\ \bar{W}(k)}} \tag{A.24}$$

The dynamics of the deviation x(k) are approximately governed by

$$x(k+1) = \left[f_k x_1 \; f_k x_2 \ldots f_k x_n \right] x(k) + w(k) \tag{A.25}$$

where the initial deviation x(0) has zero mean and covariance matrix P(0) and where $w(k) = [f_k w_1 \; f_k w_2 \; \ldots \; f_k w_n]\,(W(k) - \bar{W}(k))$ has zero mean and co-

variance matrix Q(k). Note that the bracketed quantities are matrices because $f_k x_i$ and $f_k w_i$ are vectors. By making the correspondence

$$\Phi_k \equiv \left[f_k x_1 \; f_k x_2 \; \cdots \; f_k x_n \right] \tag{A.26}$$

it is seen that Equation (A.25) is a linear difference equation of the form of Equation (A.1).

The measurement equation (assuming that the measurements are linear combinations of the state variables) is of the form

$$Y_{mk} = C_m X(k) + r_{mk}. \tag{A.27}$$

Upon substitution of Equation (A.23) into (A.27),

$$Y_{mk} = C_m[x(k) + Xnom(k)] + r_{mk} \tag{A.28}$$

or,

$$y_{mk} = Y_{mk} - C_m Xnom(k) = C_m x(k) + r_{mk}. \tag{A.29}$$

Note that once the measurement Y_{mk} is available, the pseudo-measurement y_{mk} can be computed and is of the form (A.4). In the linearized Kalman filter, Equation (A.25) is interpreted as the model of the physical system and the conditional mean of the deviation $\hat{x}(k)$, and its error covariance matrix is computed as earlier in this section. Once x(k) has been computed, Equation (A.23) is employed to compute the state estimate

$$\hat{X}(k) = Xnom(k) + \hat{x}(k). \tag{A.30}$$

SUMMARY OF THE KALMAN FILTER AND MEASUREMENT STRATEGY OPTIMIZATION

The procedures described in this appendix can be employed to estimate the state of any physical system for which an uncertain nonlinear model and noisy measurements are available. The steps in this procedure are as follows:

(1) Model the system and determine the necessary statistics of the initial state and model uncertainty.

(2) Compute the nominal state.

(3) Linearize the nonlinear model about the nominal.

(4) Optimize the measurement strategy and controllable model error covariance matrix.

(5) Compute the estimation error covariance matrix.

(6) Collect and process the measurements to compute the estimate of the deviation.

(7) Compute the estimate of the state.

APPENDIX B

OPTIMAL MEASUREMENT STRATEGY: OVERVIEW OF COMPUTER PROGRAM

This program computes the minimum dollar cost measurement strategy subject to satisfaction of specified limits on the diagonal elements of the state covariance matrix at each event time. The theoretical details are presented in DePalma (1977). An example of the usage of this program is presented in Section 5.

DESCRIPTION

This program optimizes measurement strategy for the discrete time problem using linearized Kalman filter techniques. The method is described in Appendix A. Briefly, given the following system

$$x = \Phi_{k-1}x_{k-1} + B_{k-1}w_{k-1} + B_{k-1}f_{k-1} \tag{B.1}$$

$$z_k = H_k x_k + v_k \tag{B.2}$$

where x_k is an n-dimensional state vector, w_k is an n-vector of process noise, f_k is an m-dimensional input vector, z_k is an ℓ-dimensional measurement vector, and v_k is an ℓ vector of measurement noise. Φ_{k-1} (the state transition matrix) and B_{k-1} are known n x n matrices, and H_{k-1} is a known ℓxn matrix. In addition, the statistics of w_k and v_k are known

$$E\left[w_k\right] = 0,\ E\left[w_k w_k^T\right] = Q_k\ , \tag{B.3}$$

$$E\left[v_k\right] = 0,\ E\left[v_k v_k^T\right] = R_k\ . \tag{B.4}$$

Then, the covariance matrix P_k for the above system processed by a Kalman filter can be calculated as follows:

$$P_k^- = \Phi_{k-1}P_{k-1}\Phi_{k-1}^T + B_{k-1}Q_{k-1}B_{k-1}^T \tag{B.5}$$

$$P_k^+ = (I - K_k H_k)P_k^- \tag{B.6}$$

where

$$K_k = P_k^- H_k^T(H_k P_k^- H_k^T + R_k)^{-1}. \tag{B.7}$$

This is the Kalman gain. This program determines r_k, $r_{min} \leq r_k$, such that the economic cost

$$\sum_{k=1}^{K} \frac{c_k}{r_k} \quad , \quad (c_k \text{ a known measurement cost factor}) \tag{B.8}$$

is minimized subject to inequality constraints on the diagonal elements of the covariance matrix.

PROBLEM FORMULATION

The first step in optimizing a measurement strategy with this program is to convert the system under consideration into a form useable by the program. For a general continuous time problem with $\dot{X} = F(t,X,f)$, X an n-vector:

1. Form the linearized problem using a Taylor series, that is, let $x(t) = X(t) - X_{nom}(t)$ where $X_{nom}(t)$ is the nominal trajectory.

Then

$$\dot{X}(t) \cong \left[\frac{\partial F}{\partial X}\right]_{X_{nom}(t)} x(t) \equiv A(t)x(t) \tag{B.9}$$

For the interval of interest $[0,\tau]$, form k subdivisions of length Δt, that is, $\Delta t = \tau/k$, where k is selected by accuracy considerations. Then the k state transition matrices $\Phi_1, \ldots, \Phi_k$ are defined by the series

$$\Phi_1 = I + \frac{A(0)\Delta t}{1!} + \frac{A(0)^2\Delta t^2}{2!} + \ldots + \frac{A^{n_1}(0)\Delta t^{n_1}}{n_1!} \tag{B.10}$$

$$\Phi_k = I + \frac{A[(k-1)*\Delta t]\Delta t}{1!} + \frac{A[(k-1)*\Delta t]^2\Delta t^2}{2!} + \ldots + \frac{A[(k-1)*\Delta t]^{n_k}\Delta t^{n_k}}{n_k!} \tag{B.11}$$

where n_i is selected such that

$$\left\| \Phi_i^{n_i} - \Phi_i^{n_i-1} \right\| \leq \varepsilon \qquad \text{(a prespecified small number).}$$

2. Determine $Q(t) = E[w\ w^T]$ where w is an n-vector of process noise. Then form k nxn matrices (diagonal)

$$W_o(n) = Q(n \cdot \Delta t);\ n = 1, \ldots, k. \tag{B.12}$$

3. The program permits the control of the diagonal matrix W_o by measurements such that $W_o = W_{max}$ for no measurements, and $W_o = W_{min}$ for maximum permissible measurements. If the problem being considered will use M such measurements, then form the two M-vectors W_{min} and W_{max} for the M measurements, where the W_{min} and W_{max} vectors define the diagonal elements of the W_{min} and W_{max} matrices.

4. Determine the ℓ vector R_{min}, which is the diagonal of $E[v\ v^T]$ for maximum permissible measurements.

5. Determine the cost vectors β_W and β_R such that is maximum permissible measurements are made, then the total cost is

$$\sum_{i=1}^{k} \left[\sum_{j=1}^{m} \beta_{W_j} \cdot \frac{1}{W_{min_j}} + \sum_{n=1}^{\ell} \beta_{R_n} \cdot \frac{1}{R_{min_n}} \right] \tag{B.13}$$

where β_W and β_R are the same for each time k.

6. Determine $P_o = E\left[(x_o - x_o)(x_o - x_o)^T\right]$, that is, the initial state covariance matrix.

7. Determine the k n-vectors P_{max} that are the maximum allowable variances for each state at each step.

DIMENSIONS

The program has the capability of segmenting the system being considered. For example, in the eutrophication model presented in Section 6, a basin is divided into five segments, all with similar state equations. For a single segment there are eight state variables (8 trophic levels) and seven parameters for identification. Each of the eight states is measured, but none of the functions is measured. Then, for each segment:

$$N = 15,\ \ell = 8,\ M = 0.$$

For the total problem:

$$N = 75,\ \ell = 40,\ M = 0.$$

In the lake problem of Section 5 there is one segment, two state variables, two forcing functions to be measured and identified, and the state variables are to be measured. Then,

N = 3, ℓ = 2, M = 2.

In the program coding, the following integers are defined:

NT = K	(the number of time steps)
NSEG	(the number of segments)
NSS = N/NSEG	(the number of state variables per segment)
NSR = ℓ/NSEG	(the number of state measurements per segment)
NSW = M/NSEG	(the number of forcing function measurements per segment)
NS = N	(the total number of state variables)
NR = ℓ	(the total number of state measurements)
NW = M	(the total number of forcing function measurements)

(Note: NSS*NSEG = NS, NSR*NSEG = NR, and NSW*NSEG = NW.)

The program must be dimensioned for each new problem since the amount of core storage required is a function of $N^2 \cdot NT$. The matrices should be dimensioned as follows:

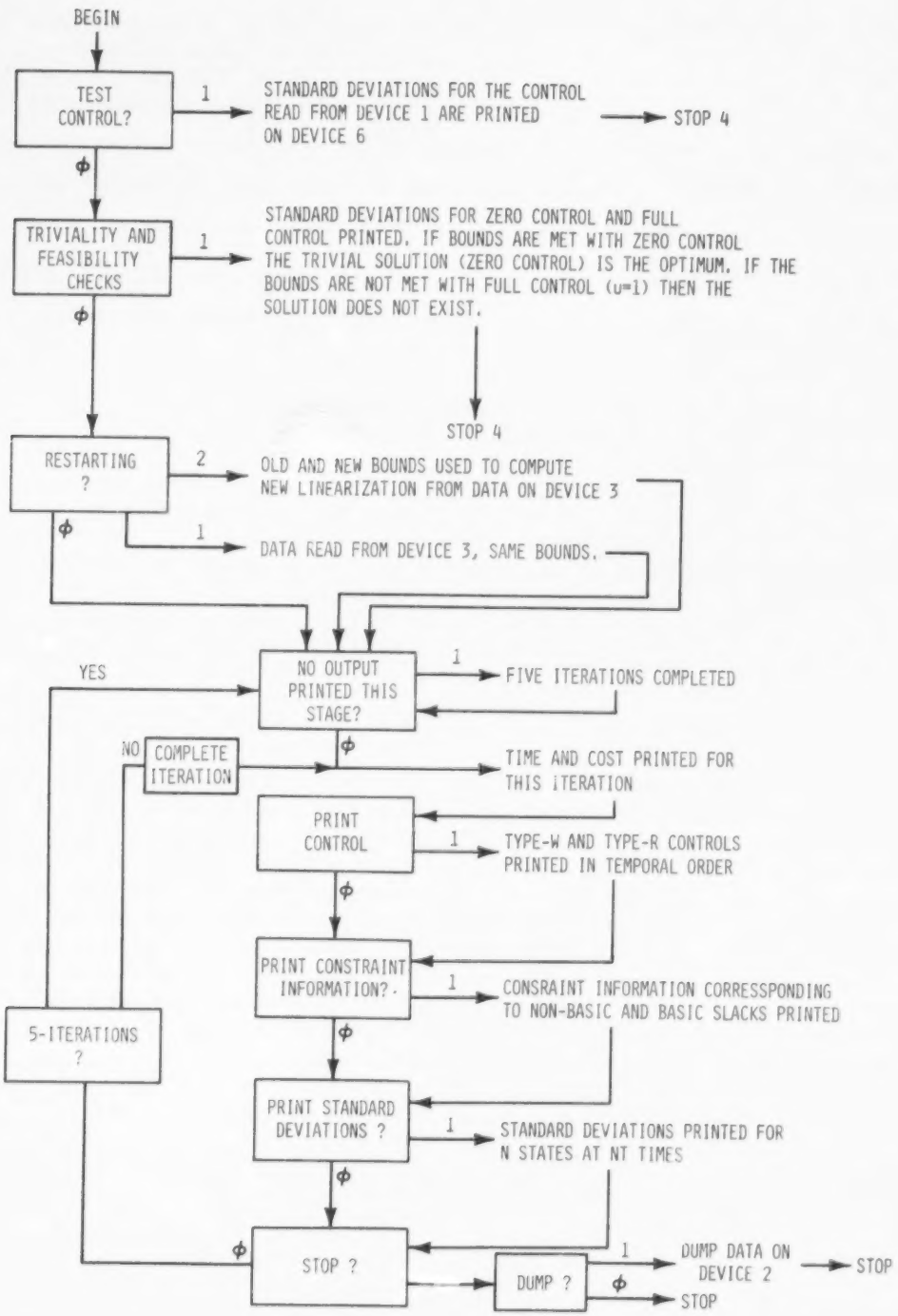
MATRIX	DIMENSION
STNUMW, BETAW, WMIN, WMAX	(NW)
STNUMR, RMIN, BETAR	(NR)
PMAX, PMAXO	(NT, NS)
PO, TEM, D, PINVM, PM, PINV, P, PHIP	(NS, NS)
WO, PHI, E, SAVE	(NS, NS, NT)

FORMAT	SYMBOL	DESCRIPTION
75E12.5	PHI(I,J,N)	The NT state transition matrices starting from time = 0 and read row by row
75E12.5	WO(I,J,N)	The NT process noise matrices (diagonal) read in same order as PHI(I,J,N)
4015	STNUMW(I)	The NW locations of the measured forcing functions within the state vector. For example, if NS = 4 and NW = 2, and the forcing functions are measured on the first and third states, then STNUMW(1) = 1, STNUMW(2) = 3
75E12.5	WMIN(I)	The NW minimum variances on WO
75E12.5	WMAX(I)	The NW maximum variances on WO
75E12.5	BETAW(I)	The NW cost values for full measurements

FORMAT	SYMBOL	DESCRIPTION
4015	STNUMR(I)	The NR locations of the measured state variables within the state vector. For example, if NS = 4 and second, third, and fourth states are measured, then STNUMR = 2,3,4
75E12.5	RMIN(I)	The NR minimum covariances for a maximum measurement
75E12.5	BETAR(I)	The NR cost values for full measurements
75E12.5	PO(N,N)	The initial covariance matrix read row by row.
NOTE:	if NW = 0 Skip STNUMW, WMIN, WMAX, BETAW if NR = 0 Skip STNUMR, RMIN, BETAR	
75E12.5	U(I)	The (NR + NW)*NT controls if a control is to be tested; otherwise zeros
75E12.5	PMAXO(NS,NT)	The previous N vectors of standard deviation constraints on the states if using restart feature (see program operation); otherwise, large, e.g., 1.00E + 05

PROGRAM OPERATION

The program is interactive and must be run from a terminal. The flow chart for operation is presented below. The program prints out a number of options for the user. The user either selects this option (by typing 1) or ignores it (by typing zero). During the optimization the user can terminate, continue, or dump (for restart with new bounds). He also has a choice of outputting as the optimization proceeds. Briefly, the method starts with the zero control and proceeds to the optimal control (that is, minimum cost subject to the covariance constraints). When the cost does not change for several iterates, it is assumed that the optimum has been found. The program has five iterations per stage, and the output can be controlled for an entire stage or for a single interation.


BEGIN
TEST CONTROL?
1
STANDARD DEVIATIONS FOR THE CONTROL READ FROM DEVICE 1 ARE PRINTED ON DEVICE 6
STOP 4
Φ
TRIVIALITY AND FEASIBILITY CHECKS
1
STANDARD DEVIATIONS FOR ZERO CONTROL AND FULL CONTROL PRINTED. IF BOUNDS ARE MET WITH ZERO CONTROL THE TRIVIAL SOLUTION (ZERO CONTROL) IS THE OPTIMUM. IF THE BOUNDS ARE NOT MET WITH FULL CONTROL (u=1) THEN THE SOLUTION DOES NOT EXIST.
STOP 4
Φ
RESTARTING ?
2
OLD AND NEW BOUNDS USED TO COMPUTE NEW LINEARIZATION FROM DATA ON DEVICE 3
Φ
1
DATA READ FROM DEVICE 3, SAME BOUNDS.
YES
NO OUTPUT PRINTED THIS STAGE?
1
FIVE ITERATIONS COMPLETED
NO
COMPLETE ITERATION
Φ
TIME AND COST PRINTED FOR THIS ITERATION
PRINT CONTROL
1
TYPE-W AND TYPE-R CONTROLS PRINTED IN TEMPORAL ORDER
Φ
PRINT CONSTRAINT INFORMATION?
1
CONSRAINT INFORMATION CORRESSPONDING TO NON-BASIC AND BASIC SLACKS PRINTED
Φ
5-ITERATIONS ?
PRINT STANDARD DEVIATIONS ?
1
STANDARD DEVIATIONS PRINTED FOR N STATES AT NT TIMES
Φ
Φ
STOP ?
1
DUMP DATA ON DEVICE 2
STOP
DUMP ?
Φ
STOP

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